

# *Quantum Collision Theory*

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1975

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# Preface

The purpose of this book is to give a self-contained and unified presentation of the methods of quantum collision theory, with applications to atomic, nuclear and high-energy processes. It is primarily aimed at graduate students in theoretical physics, although it is hoped that any physicist whose main interest lies in microphysics will also find it useful.

The book is divided into four parts. The first one is devoted to the presentation of the *basic definitions* and to the study of collision *kinematics*. The former is done in Chapter 1, where the various types of collisions and the concepts of channels and cross sections are defined. Chapter 2 entirely deals with kinematical questions, first in the non-relativistic case and then for relativistic collisions.

The second part (Chapters 3–12) contains a detailed discussion of the simplest collision problem, namely the non-relativistic scattering of two particles interacting through a potential which depends only on their relative coordinate. Because of its simplicity, this problem provides a good introduction to the methods of collision theory. Moreover, since “exact” solutions can often be readily obtained in this case, potential scattering is a convenient “laboratory” in which one can test approximation methods that become unavoidable in more complicated situations.

The *general features of potential scattering* are first discussed in Chapter 3. The following chapter is devoted to the *method of partial waves*, while the *Lippmann–Schwinger equation* for potential scattering is studied in Chapter 5. The particular case of the *Coulomb potential* is treated in Chapter 6. It is followed in Chapter 7 by an analysis of the potential scattering of *identical particles*. A number of important approximation methods are studied in Chapters 8–10: the *Born series* is discussed in Chapter 8, *semi-classical*

*approximations* are taken up in Chapter 9 and *variational methods* are considered in Chapter 10. The next chapter, which is of a more advanced nature, is entirely devoted to the *analytic properties of scattering amplitudes*. It provides an introduction to some of the most fruitful techniques recently used in elementary particles physics. Finally, the *time-dependent approach to potential scattering* presented in Chapter 12 paves the way for the general treatment of quantum collisions developed in Part III.

With the exception of Chapter 11 and of Section 2.2 on relativistic kinematics (which may both be studied at a later stage), the material contained in Parts I and II constitutes the basic subject matter of quantum scattering theory. Graduate students in physics may be expected to have already encountered parts of this material in various courses, but I believe that the unified approach given in this book will help them to gain a deeper understanding of the subject. I have also stressed in the first two parts the pedagogical approach to scattering theory, the beginning sections being purposely designed to have a minimum of notational complication. In the same spirit I have also included a series of problems at the end of both Parts I and II. Having mastered the basic material contained in these first two parts, the student is then prepared to go on to the more advanced topics contained in the remaining parts of the book.

The *general treatment of quantum collisions* is the subject of Part III. This part begins in Chapter 13 with general notions of *quantum dynamics*. This formalism is then applied in Chapter 14 to analyze quantum collisions from a time-dependent point of view. It leads to the central concepts of *S- and T-matrices*. The calculation of the *transition probabilities and cross sections* is carried out in Chapter 15. This chapter also contains a discussion of the Lorentz invariance of the cross sections, together with an investigation of some important consequences of the unitarity of the *S-matrix*.

Chapter 16 is devoted to the *determination of the S- and T-matrices*. It contains the derivation of the general Lippmann–Schwinger equations, together with a discussion of Born expansions, variational principles and the Low equations. The reaction matrix is then introduced and the Heitler equations are proved. The modifications necessary to treat general collisions involving identical particles are then given, and the chapter ends with a study of the role played by invariance principles in the determination of the collision matrix. Chapter 17, which concludes Part III, deals with an important application of formal scattering theory, namely the problem of *two-potential scattering*.

Part IV of the book (Chapters 18–21) is devoted to the application of the general theory developed in Part III to selected problems in atomic, nuclear and high-energy physics. *Two-body* collisions are first considered in Chapter 18, first for central forces and then for non-central interactions. Generalized partial wave expansions are obtained for the collision matrix, and a detailed

discussion is given for the case of spin zero–spin one-half scattering. The Regge pole concept introduced in Chapter 11 is also used to describe some features of two-body collisions of hadrons at high energies.

Chapter 19 deals entirely with the *three-body problem*. In particular, an introduction to the Faddeev theory is given, together with a discussion of various multiple scattering expansions. Two important problems are studied in detail: electron collisions with atomic hydrogen and high-energy hadron–deuteron scattering. In the next chapter the *optical potential* method is presented and applied to high-energy hadron–nucleus scattering and to the elastic scattering of charged particles by atoms. Finally, in Chapter 21, a few typical *multiparticle scattering processes* are considered, such as electron–helium collisions and nuclear stripping or pick-up reactions. Also discussed in the last chapter is the theory of final state interactions.

This book is the outgrowth of lectures which I have given at the Universities of California (Berkeley), Brussels and Louvain over the past nine years. I wish to thank my colleagues and students at these institutions for numerous fruitful discussions and remarks. I am particularly indebted to Professor F. W. Byron, Jr. for a careful reading of the manuscript and for many helpful suggestions and comments. The proofreading of the manuscript by Dr. E. H. Mund and Dr. K. H. Winters has been of great help. It is also a pleasure to thank Mr. C. Depraetere, who drew most of the figures of this book, and Mmes G. Janssens, T. Köke, G. Mobergs and E. Péan for their expert and careful typing of the final manuscript.

CHARLES J. JOACHAIN

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# **PART I**

## **DESCRIPTION OF COLLISION PROCESSES**

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# Basic Definitions

This chapter contains a simple, descriptive introduction to quantum collision processes. We first classify the various types of collisions in Section 1.1. The concept of channel is then introduced in Section 1.2 and the cross sections are defined in Section 1.3.

## 1.1. Types of collisions

Let us consider a typical collision experiment which is illustrated by the schematic drawing of Fig. 1.1. A beam of particles A, well collimated and nearly monoenergetic, is directed towards a target. The incident beam should be neither too intense – so that the interaction between the incident particles may be neglected – nor too weak, because one wants to observe a reasonable number of “events” during the experiment.

The target usually consists of a macroscopic sample containing a large number of scatterers B. The distances between these scatterers are in general

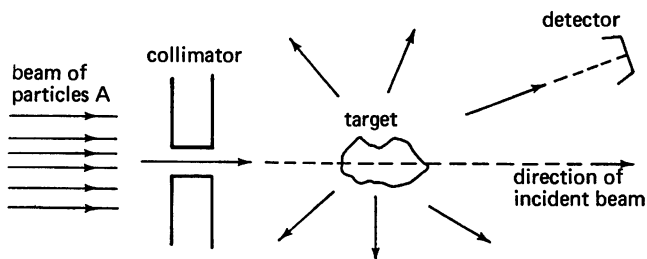


Fig. 1.1. Schematic drawing of a collision process.

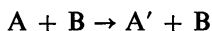
quite large with respect to the de Broglie wavelength of the incident particle, in which case one can neglect coherence effects between the waves scattered by each of the scattering centers [1]. In addition, if the target is sufficiently thin, multiple scattering by several scatterers can be neglected. One may then consider that each scatterer B acts as if it were alone, and focus one's attention on the study of a typical collision between a particle A of the incident beam and a scatterer B of the target [2].

After the collision, some or all outgoing particles are registered by detectors [3], located at a macroscopic distance from the target. Several processes can occur:

1) *Elastic scattering*: the two particles A and B are simply scattered without any change in their internal structure,



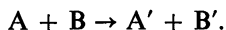
2) *Inelastic scattering*: the two particles A and B undergo a change of their internal quantum state during the collision process [4]. Denoting by A' and B' these new internal states, we may have



or



or



3) *Reactions*: the composite system (A + B) splits into two particles different from A and B, or into  $n > 2$  particles. That is,



or

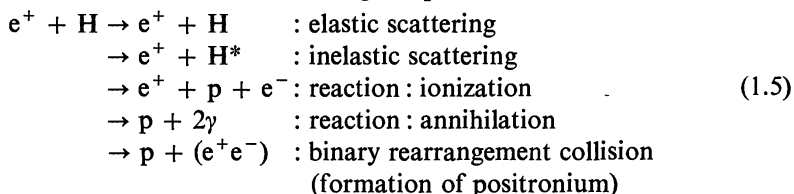


It is convenient at this point to define the terms “elementary” and “composite” particles. Since the rigorous definition of an “elementary particle” is presently rather arbitrary we shall use a practical definition and decide that *a particle is elementary if, in the particular phenomenon under study we may suppose that it is not a bound system of other particles*. For example, in low energy atomic collisions the atomic nuclei may be considered as elementary, while they appear as composite structures in nuclear reactions.

Let us now return to the reaction (1.3). If the particles A, B, C and D are all “elementary”, we shall call this process a *two-body reaction*. If on the contrary the particles A and (or) B are composite so that the reactions (1.3) and (1.4) occur because of the *exchange* of one or several elementary constituents, we shall call these processes *rearrangement collisions*. Chemical reactions are rearrangement collisions between atoms, ions and molecules; nuclear reactions are rearrangement collisions between atomic nuclei. In particular, we shall call *binary* rearrangement collisions those of the type (1.3), where two particles emerge in the final state.



As an illustration of these various types of collision processes, consider a positron  $e^+$  incident on an hydrogen atom in its ground state, for energies above the ionization threshold. Among the processes which can occur are



where  $H^*$  denotes an hydrogen atom in an excited state,  $p$  is a proton,  $e^-$  an electron,  $\gamma$  a photon and  $(e^+e^-)$  represents positronium, a bound state of the electron-positron system.

In many experimental situations it is difficult to keep track of all the outgoing particles. For example, in high energy collisions of hadrons [5], neutral particles are difficult to detect. Therefore, following Feynman [6], it is convenient to define *exclusive experiments*, where the nature and momenta of *all* outgoing particles are measured, and *inclusive* experiments where only some of the outgoing particles are detected. For example the two-body reaction (1.3) is an exclusive experiment, whereas the reaction



– where the particle  $C$  is produced together with some other outgoing particles – is an inclusive reaction.

Before we conclude this section, it is worth pointing out that many experimental settings may differ appreciably from the simple one shown in Fig. 1.1. For example, in experiments with colliding beams (as in the case of “intersecting storage rings”), crossed beams [e.g. 7] or merged beams [e.g. 8], the target itself consists of a beam of particles  $B$ . We shall return to this question in Chapter 2.

## 1.2. Channels

A channel is a possible mode of fragmentation of the composite system  $(A + B)$  during the collision. It is characterized by the number and the nature of the fragments into which the system  $(A + B)$  can be decomposed. For example, we have listed above in (1.5) five possible final channels into which the composite system  $(e^+ + H)$  may dissociate. The definition of the channels contains some arbitrariness, related to our way of specifying the precise “nature” of the fragments. For example, in the inelastic process

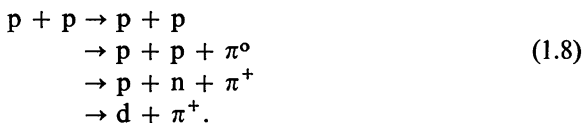


we may consider each of the excited states  $H^*$  as corresponding to a different channel, or group them into one “inelastic” channel. Ambiguities of this type

also arise in particle physics, where two particles may often be equally well considered as “different”, or “different states” of a same particle.

One of the possible modes of fragmentation of the system gives back the two original particles A and B, i.e. the initial channel. In an elastic collision, the two colliding particles remain in the initial channel. A channel is *open* if the corresponding collision is allowed by known conservation laws (energy conservation, charge conservation, etc.). Otherwise it is *closed*.

As an example, consider proton–proton scattering at energies below the threshold for production of two pions. Four possible open final channels are then



### 1.3. Cross sections. Laboratory and center of mass systems

The results of collision experiments are usually expressed in terms of characteristic quantities called *cross sections*. They are defined as follows:

*The cross section of a certain type of event in a given collision is the ratio of the number of events of this type per unit time and per unit scatterer, to the relative flux of the incident particles with respect to the target.*

To illustrate this definition, let us first consider the case of *total cross sections*. We assume that the initial channel consists of two particles A and B which are both in well defined quantum states [2]. We also suppose that the incident beam of particles A satisfies the physical requirements stated in Section 1.1. Thus a sufficiently large (but not too large) number  $N_A$  of particles A reach per unit time the target (made of particles B) with nearly parallel directions and a kinetic energy distribution sharply peaked about a given value. Let us denote by  $\mathcal{N}_A$  the average number of particles A per unit volume in the incident beam and by  $v_i$  the average magnitude of their velocity with respect to the target. The flux  $\Phi_A$  of incident particles relative to the target (i.e. the number of particles A crossing per unit time a unit area perpendicular to the direction of the incident beam and at rest with respect to the target) is then given by

$$\Phi_A = \mathcal{N}_A v_i = N_A/S \tag{1.9}$$

where  $S$  is the cross-sectional area of the incident beam, as shown in Fig. 1.2.

Next, let us assume that the target is sufficiently thin and denote by  $n_B$  the number of particles B within the “effective” target volume interacting with the incident beam. For example, if we imagine the target to be a very thin layer of thickness  $l$  perpendicular to the incident beam (see Fig. 1.2) we have

$$n_B = S \cdot l \cdot \mathcal{N}_B = S \hat{\mathcal{N}}_B \tag{1.10}$$

where  $\mathcal{N}_B$  is the number of particles B per unit volume in the target and  $\hat{\mathcal{N}}_B = \mathcal{N}_B l$  is the (average) *surface density* of the target particles.

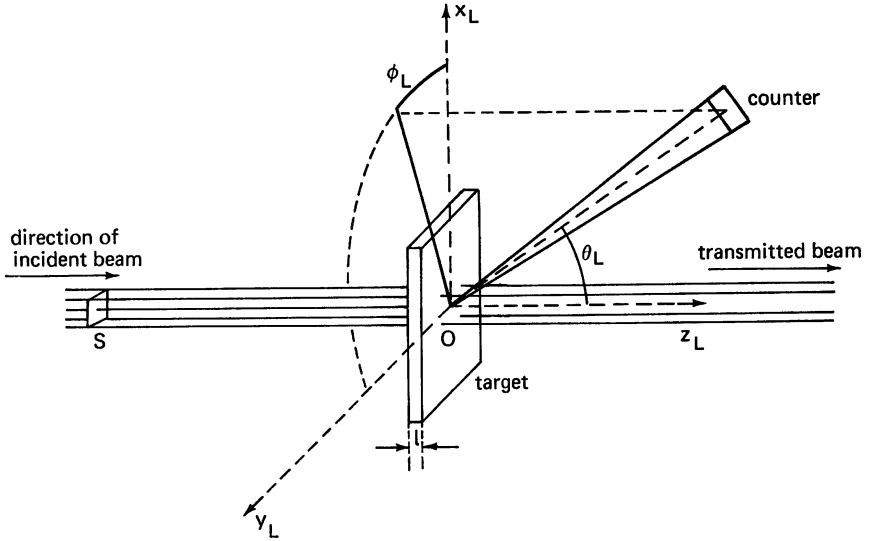


Fig. 1.2. Illustration of various quantities used in the definition of cross sections.

Let us now denote by  $N_{\text{tot}}$  the total number of particles A which have interacted per unit time with target scatterers. Under the experimental conditions assumed here, the quantity  $N_{\text{tot}}$  is directly proportional to the relative incident flux  $\Phi_A$  and the number  $n_B$  of target scatterers. We may then write

$$N_{\text{tot}} = \Phi_A n_B \sigma_{\text{tot}}. \quad (1.11)$$

According to the definition given above, the quantity  $\sigma_{\text{tot}}$  is called the *total cross section* for scattering of the particle A by the particle B. We note from eq. (1.11) that  $\sigma_{\text{tot}}$  has the dimension of an area. We also remark that if we define

$$P_{\text{tot}} = N_{\text{tot}}/N_A \quad (1.12)$$

as the total probability that an incident particle has interacted with a target scatterer and has therefore been removed from the incident beam, then by using eqs. (1.9)–(1.11) we have

$$P_{\text{tot}} = \hat{\mathcal{N}}_B \sigma_{\text{tot}}. \quad (1.13)$$

We emphasize that the definition (1.11) of  $\sigma_{\text{tot}}$  only holds for the case of a thin target (such that  $P_{\text{tot}} \ll 1$ ). Corrections must be applied when this condition is not satisfied [9].

It is important to note that in contrast with  $P_{\text{tot}}$  which depends upon various experimental parameters (such as the values of  $N_A$ ,  $\mathcal{N}_B$ ,  $\hat{\mathcal{N}}_B$ ,  $l$ ), the

quantity  $\sigma_{\text{tot}}$  depends only on the energy of the collision and refers to an intrinsic, microscopic property of the quantum system ( $A + B$ ). It gives a measure of the tendency of the particles  $A$  and  $B$  to interact at a given energy. In fact, we may consider  $\sigma_{\text{tot}}$  as an "effective area" which picks up a certain amount of the incident beam [10].

Having defined the total, complete cross section, let us now introduce total [11] cross sections corresponding to various particular processes. For example, in the case of elastic scattering, we write

$$N_{\text{tot}}^{\text{el}} = \Phi_A n_B \sigma_{\text{tot}}^{\text{el}}. \quad (1.14)$$

Here  $N_{\text{tot}}^{\text{el}}$  is the total number of particles  $A$  which have been scattered elastically per unit time and  $\sigma_{\text{tot}}^{\text{el}}$  is the total elastic cross section. Of course, if only elastic scattering between the particles  $A$  and  $B$  can happen at the particular collision energy considered, then  $\sigma_{\text{tot}} = \sigma_{\text{tot}}^{\text{el}}$ . In general, however, other collision processes can occur. In this case one defines the quantity

$$\sigma_{\text{tot}}^{\text{r}} = \sigma_{\text{tot}} - \sigma_{\text{tot}}^{\text{el}} \quad (1.15)$$

which corresponds to all non-elastic collision processes and is often called the *total reaction cross section*.

When several channels are open, the quantity  $\sigma_{\text{tot}}^{\text{r}}$  is itself a sum of cross sections corresponding to particular non-elastic processes. For example if the two-body reaction (or binary rearrangement collision)



is allowed, we may associate with it a total cross section  $\sigma_{\text{tot}}(A + B \rightarrow C + D)$  by counting all the particles  $C$  which, together with the particles  $D$ , have been produced per unit time in the collision between the beam particles  $A$  and the target particles  $B$ . Calling  $N_{\text{tot}}^{\text{C}}$  this number, we have

$$N_{\text{tot}}^{\text{C}} = \Phi_A n_B \sigma_{\text{tot}}(A + B \rightarrow C + D). \quad (1.17)$$

We shall not discuss here the problems raised by the experimental determination of the total cross sections (i.e. the measurement of the quantities  $\Phi_A$ ,  $n_B$ ,  $N_{\text{tot}}$ ,  $N_{\text{tot}}^{\text{el}}$ , etc.). We simply mention that the total (complete) cross section  $\sigma_{\text{tot}}$  may be obtained by performing an attenuation measurement, in which the intensity of the transmitted beam is compared with that of the incident beam. However, since the area of counters is finite, it is not possible in practice to distinguish between incident particles which have been scattered elastically through very small angles  $\theta$  and those which have experienced no interaction. Thus the number of particles counted in the transmitted beam also accounts for particles which have been scattered elastically near the forward direction. A possible way of eliminating this difficulty is to perform several measurements at smaller and smaller solid angles and to extrapolate to the value  $\theta = 0$ . Let us denote by  $N_{\text{T}}$  the extrapolated value of the number

of transmitted particles per unit time corresponding to the number  $N_A$  of incident particles per unit time. Then, since  $N_{\text{tot}} = N_A - N_T$  we may use eqs. (1.12) and (1.13) to write for a thin target

$$P_{\text{tot}} = 1 - N_T/N_A = \hat{\mathcal{N}}_B \sigma_{\text{tot}} \quad (1.18)$$

so that  $\sigma_{\text{tot}}$  may be deduced from the knowledge of  $N_A$ ,  $N_T$  and  $\hat{\mathcal{N}}_B$ . We note that the quantity  $N_T/N_A$  is simply the *transmission probability* through the layer [12].

The total cross sections which we have considered so far provide useful information about the interactions experienced by the colliding particles. However, more detailed insight into the nature of these interactions may be gained if *differential cross sections* are known.

Suppose, for example, that with the help of counters placed at a given (macroscopic) distance from the target, we are able to measure the number of particles of a certain kind (produced in the collision of “beam” particles A with “target” particles B) which emerge from the collision region in different directions. To analyze this *angular distribution*, we first have to choose a coordinate system or reference framework. Two very convenient choices, which are frequently used in the description of collision processes are the *laboratory (L) system* and the *center of mass (C.M.) system*. The laboratory system is the framework in which the target particle B is at rest before the collision. In what follows we shall use the subscript L to denote quantities expressed in that system. The center of mass system or *barycentric system* is defined as that coordinate system in which the center of mass of the composite system (A + B) is at rest. In both systems we assume that the z-axis has been chosen to be parallel to the incident direction.

We shall study at length in Chapter 2 the relationships between various quantities expressed in the laboratory and in the center of mass systems. For the moment, we note that *observations* are often made in the laboratory system (with important exceptions such as colliding beam experiments). As an example, we have represented in Fig. 1.2, for a typical experiment, the laboratory system  $Ox_L y_L z_L$  together with the polar angles  $(\theta_L, \phi_L)$  which define a “laboratory” direction  $\Omega_L$ . *Calculations*, on the contrary, are often performed in the center of mass system, since the three degrees of freedom attached to the center of mass of the system (A + B) may then be ignored.

Let us now return to the analysis of *angular distributions* and the definition of differential cross sections. We consider first the case of elastic collisions and work in the laboratory system. Let  $dN_{\text{el}}$  be the number of particles A scattered elastically per unit time within a solid angle  $d\Omega_L$  centered about a direction  $(\theta_L, \phi_L)$ , as shown in Fig. 1.2. Then, for a sufficiently thin target, we have [compare with eq. (1.14)]

$$dN_{\text{el}} = \Phi_A n_B \sigma_{\text{el}}(\theta_L, \phi_L) d\Omega_L. \quad (1.19)$$

The proportionality factor  $\sigma_{el}(\theta_L, \phi_L)$  is called the laboratory *differential cross section* for elastic scattering. We shall also write

$$\sigma_{el}(\theta_L, \phi_L) = \frac{d\sigma_{el}}{d\Omega_L}(\theta_L, \phi_L). \quad (1.20)$$

Since the quantity  $\Phi_A$  represents the *relative* flux of the projectile with respect to the target, we may readily transpose the definition (1.19) to the center of mass system. Thus, if  $\Omega \equiv (\theta, \phi)$  refers to the direction of emission of particle A in the center of mass system when this particle is scattered in the direction  $\Omega_L \equiv (\theta_L, \phi_L)$  in the laboratory system, we have

$$dN_{el} = \Phi_A n_B \sigma_{el}(\theta, \phi) d\Omega \quad (1.21)$$

where

$$\sigma_{el}(\theta, \phi) = \frac{d\sigma_{el}}{d\Omega}(\theta, \phi) \quad (1.22)$$

is the *center of mass differential cross section for elastic scattering*. Upon comparison of eqs. (1.19) and (1.21) we deduce that

$$\frac{d\sigma_{el}}{d\Omega_L}(\theta_L, \phi_L) d\Omega_L = \frac{d\sigma_{el}}{d\Omega}(\theta, \phi) d\Omega. \quad (1.23)$$

The *total* elastic cross section  $\sigma_{tot}^{el}$  is simply obtained by integrating the elastic differential cross section over all scattering angles. From eq. (1.23) we see that [13]

$$\sigma_{tot}^{el} = \int \frac{d\sigma_{el}}{d\Omega_L}(\theta_L, \phi_L) d\Omega_L = \int \frac{d\sigma_{el}}{d\Omega}(\theta, \phi) d\Omega \quad (1.24)$$

and we verify that  $\sigma_{tot}^{el}$  is independent of the reference frame, as any total cross section should.

The above discussion of differential cross sections may be directly generalized to the case of two-body reactions (or binary rearrangement collisions) of the type (1.16). Thus, if  $dN_C$  is the number of particles C emitted per unit time into the laboratory solid angle  $d\Omega_L$  (centered about the direction  $\theta_L, \phi_L$ ), the corresponding laboratory differential cross section is given by

$$\frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) = \frac{dN_C}{\Phi_A n_B d\Omega_L} \quad (1.25)$$

while in the center of mass system

$$\frac{d\sigma_C}{d\Omega}(\theta, \phi) = \frac{dN_C}{\Phi_A n_B d\Omega}. \quad (1.26)$$

Again we have

$$\frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) d\Omega_L = \frac{d\sigma_C}{d\Omega}(\theta, \phi) d\Omega \quad (1.27)$$

and the total cross section  $\sigma_{\text{tot}}^C \equiv \sigma_{\text{tot}}(A + B \rightarrow C + D)$  is given by

$$\sigma_{\text{tot}}^C = \int \frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) d\Omega_L = \int \frac{d\sigma_C}{d\Omega}(\theta, \phi) d\Omega. \quad (1.28)$$

Until now we have considered differential cross sections which characterize the number of particles emitted into a solid angle centered about a direction defined by polar angles. In certain situations it is convenient to use different kinematical variables, as we shall illustrate in Chapter 2 for the case of two-body relativistic collisions. The corresponding differential cross sections are then readily defined by analogy with the above discussion. For reactions with more than two particles in the final state a variety of differential cross sections may be introduced, since the number of kinematical variables necessary to describe the collision grows rapidly with the number of particles present in the final state. We shall also consider this problem in Chapter 2.

We now return to the basic definition of cross sections given at the beginning of this section. Since this definition and the subsequent discussion [see for example eqs. (1.11), (1.17) or (1.19)] imply that the cross sections are independent of the number of incident particles striking the target per unit time, we may choose this number to be equal to one. Therefore the cross sections may be equally considered as *transition probabilities per unit time, per unit target scatterer and per unit relative flux of the incident particles with respect to the target*.

In atomic physics, where the scattering centers have linear dimensions of the order of  $1\text{\AA} = 10^{-8}\text{ cm}$ , one usually uses as the unit of length the “radius of the first Bohr orbit” of the hydrogen atom, namely

$$a_0 = 5.29 \times 10^{-9}\text{ cm}.$$

Using this *atomic unit* of length, the cross sections are expressed in units of  $a_0^2 = 2.80 \times 10^{-17}\text{ cm}^2$  [14].

In nuclear and particle physics, where the scattering centers have linear dimensions of the order of 1 fermi  $\equiv 1\text{ fm} = 10^{-13}\text{ cm}$ , one measures the cross sections in  $\text{fm}^2$ , in barns or in millibarns, where

$$1\text{ barn} \equiv 1\text{ b} = 10^{-24}\text{ cm}^2 = 10^2\text{ fm}^2,$$

$$1\text{ millibarn} \equiv 1\text{ mb} = 10^{-27}\text{ cm}^2.$$

## References and notes

- [1] Diffraction processes in crystals such as the diffraction of electrons, thermal neutrons or X rays provide important exceptions to this rule.
- [2] For simplicity, we shall first confine ourselves to the study of an “individual” collision between a beam particle A and a target particle B, assuming that the quantum system (A + B) may be described by a single state vector in Hilbert space (see Appendix A). Scattering systems in mixed states will be considered in Section 15.5.

- [3] We shall not attempt to describe the experimental aspects of the detection process. The detection system will simply be represented schematically by a "counter" which records outgoing particles.
- [4] This change could be a simple modification of the spin orientation of the particles. In this case, however, and because there is no change in the internal energy of the particles, we shall follow the usual terminology and rank these collisions among the elastic ones.
- [5] The word "hadron" denotes the strongly interacting particles (baryons and mesons).
- [6] FEYNMAN, R. P. (1969), *Phys. Rev. Letters* **23**, 1415; see also FEYNMAN, R. P. (1969), in *High Energy Collisions*, Proc. Third Int. Conf., Stony Brook, Sept. 1969 (Gordon and Breach, New York) p. 237.
- [7] FITE, W. C., A. C. H. SMITH and R. F. STEBBINGS (1962), *Proc. Roy. Soc.* **A268**, 527.
- [8] NEYNABER, R. H. (1969), Experiments with Merging Beams, in *Advances in Atomic and Molec. Physics*, eds. D. R. Bates and I. Estermann, Vol. 5 (Academic Press, New York) p. 57.
- [9] For example, if the target contains  $\mathcal{N}_B$  particles per unit volume and has a thickness  $l$  (measured in the direction parallel to the incident beam) then eq. (1.13) may be generalized to read

$$P_{\text{tot}} = N_{\text{tot}}/N_A = 1 - \exp(-\mathcal{N}_B/\sigma_{\text{tot}}) \quad (1.13')$$

provided that "repopulation" effects of the incident beam through collisions may be neglected. Evidently eq. (1.13') reduces to eq. (1.13) for a sufficiently thin target such that  $\mathcal{N}_B/\sigma_{\text{tot}} = \hat{\mathcal{N}}_B \sigma_{\text{tot}} \ll 1$ .

- [10] It should not be inferred from this simple interpretation that total cross sections may be directly associated with "geometric" properties of the colliding particles. We shall see for example that cross sections may vary very significantly over short colliding energy ranges.
- [11] The adjective "total" is used here by contrast with the term "differential" defined below.
- [12] For a target of thickness  $l$  we may use the result (1.13') of [9] to write the transmission probability  $N_T/N_A$  as

$$N_T/N_A = \exp(-\mathcal{N}_B/\sigma_{\text{tot}}), \quad (1.18')$$

- [13] We shall often use the symbol  $\int d\Omega$  to denote  $\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta$ , where the direction  $\Omega$  is characterized by the polar angles  $(\theta, \phi)$  and we recall that  $d\Omega = \sin \theta d\theta d\phi$ .
- [14] Total atomic cross sections are also often expressed in units of  $\pi a_0^2 = 8.80 \times 10^{-17} \text{ cm}^2$ .



# Kinematics

The purpose of collision *kinematics* – by contrast with *dynamics* – is to study collision phenomena independently of the interactions which induce them. One of the most important of these kinematical problems consists in transforming the results of calculations or measurements from one frame of reference to another. This will be done first for non-relativistic collisions and then for relativistic processes. All we shall use, in fact, will be the conservation of momentum and energy together with the transformation laws from one system of reference to the other. We devote particular attention to the case of two-body reactions for which, in the relativistic case, we introduce the Mandelstam variables [1]. We also consider briefly relativistic collisions with three or more particles in the final state, and define some variables which are particularly useful in describing such processes. More details about kinematical questions may be found for example in the books of Baldin, Goldansky and Rosental [2], Hagedorn [3] and Michalowicz [4].

## 2.1. Non-relativistic kinematics

### 2.1.1. Laboratory and center of mass systems

We have already defined in Chapter 1 the laboratory and center of mass coordinate systems. We recall these definitions here for convenience. We consider a collision between a “beam” particle A and a “target” particle B. The *laboratory system* is the framework in which the target particle B is at rest before the collision. The *center of mass (C.M.) system* or *barycentric system* is defined as that coordinate system in which the center of mass of the

composite system (A + B) is at rest. Hence, if  $\mathbf{p}_A$  and  $\mathbf{p}_B$  are the momenta of particles A and B in the C.M. system, we have

$$\mathbf{p}_A + \mathbf{p}_B = 0. \quad (2.1)$$

In what follows we shall continue to use the subscript L to denote quantities in the laboratory system. Let us choose the incident direction as the z-axis in both C.M. and laboratory systems. Calling  $\hat{\mathbf{z}}$  the unit vector along this z-axis, we denote by

$$\mathbf{V}_L = V_L \hat{\mathbf{z}} \quad (2.2)$$

the velocity of the center of mass in the laboratory system. Since the center of mass always maintains its uniform rectilinear motion, it is clear that the laboratory and C.M. systems are in uniform translational motion of velocity  $\mathbf{V}_L$  with respect to each other. Assuming that the collision between the two particles A and B is non-relativistic, one passes from the center of mass system to the laboratory system by the Galilean transformation

$$\begin{cases} \mathbf{r}_L = \mathbf{r} + \mathbf{V}_L t \\ t_L = t \end{cases} \quad (2.3)$$

or, more explicitly – with a suitable choice of x and y axis –:

$$\begin{cases} x_L = x \\ y_L = y \\ z_L = z + V_L t \\ t_L = t. \end{cases} \quad (2.4)$$

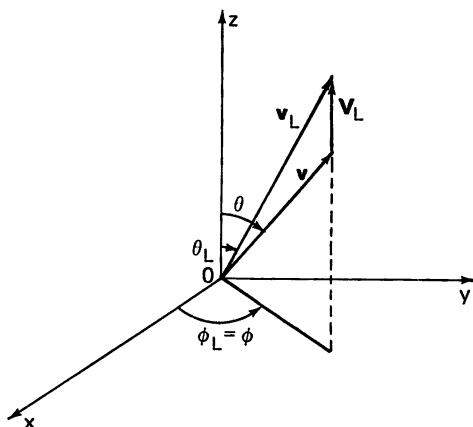


Fig. 2.1. Illustration of the velocities  $\mathbf{v}$ ,  $\mathbf{v}_L$  and  $\mathbf{V}_L$  and the angles  $(\theta, \phi)$  and  $(\theta_L, \phi_L)$  of the text.

Therefore, if  $\mathbf{v}$  is the velocity of a particle in the C.M. system, pointing in the direction  $(\theta, \phi)$ , and  $\mathbf{v}_L$  its velocity in the laboratory system, corresponding to a direction  $(\theta_L, \phi_L)$ , one has

$$\mathbf{v}_L = \mathbf{v} + \mathbf{V}_L \quad (2.5)$$

so that

$$\begin{aligned} v_L \cos \theta_L &= v \cos \theta + V_L \\ v_L \sin \theta_L &= v \sin \theta \\ \phi_L &= \phi. \end{aligned} \quad (2.6)$$

Eliminating  $v_L$  from the first two of eqs. (2.6), we obtain

$$\tan \theta_L = \frac{\sin \theta}{\cos \theta + \tau} \quad (2.7)$$

or

$$\cos \theta_L = \frac{\cos \theta + \tau}{(1 + 2\tau \cos \theta + \tau^2)^{1/2}} \quad (2.8)$$

where

$$\tau = V_L/v. \quad (2.9)$$

We shall show below how to calculate explicitly the quantity  $\tau$  as a function of the masses of the particles and of the initial and final kinetic energies associated with the relative motion in the C.M. system. For the moment, we note that the relations (2.6) suggest a simple geometrical construction [5] of  $\theta_L$  as a function of  $\theta$  which is illustrated in Fig. 2.2. We see from this figure that three cases must be considered:

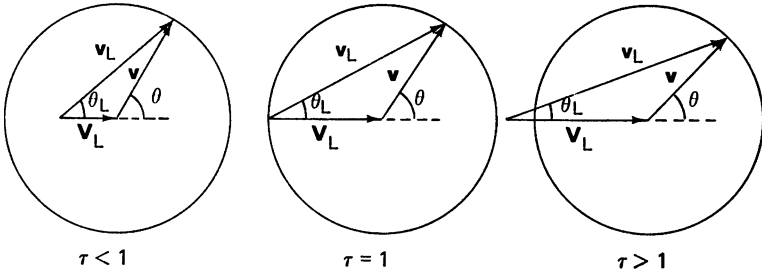


Fig. 2.2. Geometrical construction of the laboratory scattering angle  $\theta_L$  as a function of the C.M. scattering angle  $\theta$ .

1) For  $\tau < 1$ , eq. (2.7) shows that  $\theta_L$  increases monotonically from 0 to  $\pi$  as  $\theta$  grows from 0 to  $\pi$ . We also note that  $\frac{1}{2}\theta < \theta_L < \theta$ . Moreover,  $\theta_L \rightarrow \theta$  as  $\tau \rightarrow 0$ , i.e. when the C.M. coincides with the target particle and remains therefore at rest in the laboratory system.

2) If  $\tau = 1$ , then  $\theta_L = \frac{1}{2}\theta$ . In this case  $\theta_L$  varies from 0 to  $\frac{1}{2}\pi$  as  $\theta$  varies from 0 to  $\pi$ .

3) Finally, when  $\tau > 1$ ,  $\theta_L$  first grows from 0 to a maximum value  $\theta_{L \max} = \sin^{-1}(1/\tau)$ , which is less than  $\frac{1}{2}\pi$  as  $\theta$  increases from 0 to  $\cos^{-1}(-1/\tau)$ ; then  $\theta_L$  decreases to 0 as  $\theta$  grows further to reach  $\pi$ . We note that there are two values of  $\theta$  that correspond to a particular value of  $\theta_L$  between 0 and  $\sin^{-1}(1/\tau)$ . If we denote the smaller of these two values of  $\theta$  by  $\theta_<$  and the

larger by  $\theta_>$  we see from Fig. 2.2 that  $\theta_L = \frac{1}{2}(\theta_< + \theta_> - \pi)$ . We also note from this figure that the angles  $\theta_<$  and  $\theta_>$  giving rise to the same  $\theta_L$  correspond to different values of the velocity  $v_L$  of the detected particle; the larger velocity is associated with the smaller value of  $\theta$ .

What is the relation between the initial kinetic energy in the laboratory system and in the C.M. system? Since a non-relativistic particle of mass  $m$ , velocity  $\mathbf{v}$  and momentum  $\mathbf{p} = m\mathbf{v}$  has a kinetic energy  $K = \frac{1}{2}mv^2 = p^2/2m$ , the initial kinetic energy in the laboratory system is given by

$$(K_i)_L = \frac{(p_A)_L^2}{2m_A} = \frac{(P)_L^2}{2m_A}. \quad (2.10)$$

Here  $m_A$  is the mass of the particle A and  $(p_A)_L$  its momentum in the laboratory system, such that

$$(p_A)_L = (P)_L \quad (2.11)$$

where  $(P)_L$  is the total momentum in the laboratory system.

Let us now calculate the initial kinetic energy  $K_i$  available in the C.M. system. Since the center of mass is at rest in that system, we obtain  $K_i$  by subtracting from  $(K_i)_L$  the kinetic energy of the center of mass in the laboratory system. Thus, introducing the total mass  $M = m_A + m_B$ , we have

$$K_i = (K_i)_L - (P)_L^2/2M \quad (2.12)$$

where we have used the fact that the center of mass moves in the laboratory system as a free particle of mass  $M$ , momentum  $(P)_L$  and energy  $(P)_L^2/2M$ . Using eqs. (2.10) and (2.12), we also find that

$$K_i = \frac{m_B}{m_A + m_B} (K_i)_L. \quad (2.13)$$

Because the center of mass always moves as a free particle, “unconcerned” by the collision process, we see that it is the quantity  $K_i$ , namely the kinetic energy in the C.M. system, which characterizes physically the collision. For example, in electron-atom scattering, where  $m_A$ , the electron mass, is much smaller than  $m_B$ , the mass of the atom, the relation (2.13) gives

$$K_i \simeq (K_i)_L \quad (2.14)$$

so that almost all the initial kinetic energy in the laboratory system is available for the collision in the C.M. system. On the contrary, for proton-proton scattering ( $m_A = m_B$ ), we have

$$K_i = \frac{1}{2}(K_i)_L. \quad (2.15)$$

Thus, only one half of the initial kinetic energy in the laboratory system is transformed into C.M. kinetic energy, the other half being “dissipated” into the motion of the center of mass.

We shall now obtain another useful expression of  $K_i$ . We first define the

relative momentum  $\mathbf{p}$  of two particles 1 and 2 having masses  $m_1$  and  $m_2$  and momenta  $\mathbf{p}_1$  and  $\mathbf{p}_2$ . It is such that

$$\mathbf{p} = \frac{m_2 \mathbf{p}_1 - m_1 \mathbf{p}_2}{m_1 + m_2} \quad (2.16)$$

and is easily seen from eqs. (2.3) to be invariant with respect to a Galilean transformation. The initial relative momentum of two colliding particles A and B is therefore given by

$$\mathbf{p}_i = \mathbf{p}_A = -\mathbf{p}_B \quad (2.17)$$

or

$$\mathbf{p}_i = \frac{m_B}{m_A + m_B} (\mathbf{p}_A)_L. \quad (2.18)$$

In obtaining eqs. (2.17) and (2.18) we have used the definition (2.16), the momenta of the colliding particles A and B being evaluated successively in the C.M. and in the laboratory system. The kinetic energy available in the C.M. system may then be written as

$$K_i = \frac{p_A^2}{2m_A} + \frac{p_B^2}{2m_B} = \frac{p_i^2}{2\mu_i} \quad (2.19)$$

where

$$\mu_i = m_A m_B / (m_A + m_B) \quad (2.20)$$

is the reduced mass of the two particles A and B appearing in the initial channel. We verify that by using eqs. (2.18) and (2.10) in eq. (2.19) we find again the relation (2.13) between  $K_i$  and  $(K_i)_L$ .

Having studied the relationship between the C.M. and laboratory kinetic energies in the initial channel, we may easily repeat this analysis for the various final channels corresponding to the collisions listed in Section 1.1. As an example, consider the binary rearrangement collision (or two-body reaction)



In Fig. 2.3 we have represented this process in the laboratory system, while in Fig. 2.4 the collision is described in the C.M. system.

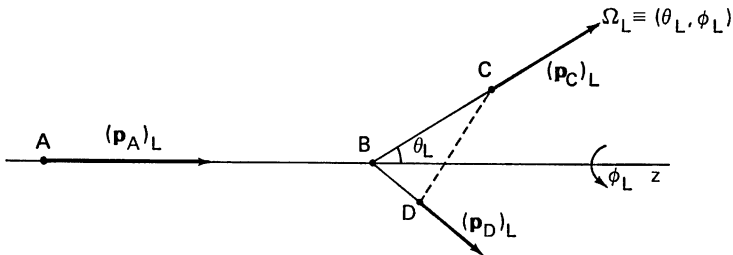


Fig. 2.3. A binary rearrangement collision or two-body reaction  $A + B \rightarrow C + D$  in the laboratory system.

The kinetic energy available in the C.M. system for the final channel is simply [6]

$$K_f = (K_f)_L - (P)_L^2/2M. \quad (2.22)$$

Here

$$(K_f)_L = (p_C)_L^2/2m_C + (p_D)_L^2/2m_D \quad (2.23)$$

is the final channel kinetic energy in the laboratory system, while

$$(P)_L = (p_A)_L = (p_C)_L + (p_D)_L \quad (2.24)$$

is the total momentum in the laboratory system.

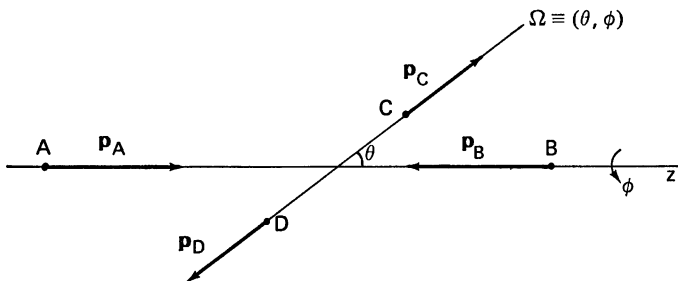


Fig. 2.4. A binary rearrangement collision or two-body collision  $A + B \rightarrow C + D$  in the center of mass system.

We also have in the C.M. system

$$P = p_A + p_B = p_C + p_D = 0 \quad (2.25)$$

so that, from eq. (2.16) we deduce that the final relative momentum is given by [compare with eqs. (2.17) and (2.18) for the initial relative momentum]

$$p_f = p_C = -p_D \quad (2.26)$$

and

$$p_f = \frac{m_D(p_C)_L - m_C(p_D)_L}{m_C + m_D}. \quad (2.27)$$

Hence, for a two-body reaction of the type (2.21), we may also write the final kinetic energy in the C.M. system as

$$K_f = p_C^2/2m_C + p_D^2/2m_D = p_f^2/2\mu_f \quad (2.28)$$

where

$$\mu_f = m_C m_D / (m_C + m_D) \quad (2.29)$$

is the reduced mass of the particles C and D appearing in the final state.

The foregoing analysis is even simpler for elastic collisions (1.1) or inelastic processes (1.2). It is more complicated, however, for reactions of the type



with more than two particles in the final state. In this case the final C.M. kinetic energy is still given by eq. (2.22), with

$$(K_f)_L = (p_1)_L^2/2m_1 + (p_2)_L^2/2m_2 + \cdots (p_n)_L^2/2m_n \quad (2.31)$$

where  $(p_1)_L, (p_2)_L, \dots (p_n)_L$  are the laboratory momenta of the  $n$  outgoing particles and  $m_1, m_2, \dots m_n$  are their masses. Furthermore, we now have

$$(\mathbf{P})_L = (\mathbf{p}_A)_L = (\mathbf{p}_1)_L + (\mathbf{p}_2)_L + \cdots (\mathbf{p}_n)_L \quad (2.32)$$

while in the C.M. system

$$\mathbf{P} = \mathbf{p}_A + \mathbf{p}_B = \mathbf{p}_1 + \mathbf{p}_2 + \cdots \mathbf{p}_n = 0. \quad (2.33)$$

It is worth noting that the simple formula (2.28) does not apply to reactions (2.30) with more than two particles in the final state, since more than one relative vector is clearly necessary in that case.

### 2.1.2. Exothermic and endothermic collisions. Thresholds

We have already applied extensively the law of conservation of momentum. We now make use of the conservation of energy. Let us consider a general reaction (2.30) with  $n \geq 2$  and denote respectively by  $w_A, w_B, w_1, w_2, \dots w_n$  the internal energies [7] of the particles A, B, C<sub>1</sub>, C<sub>2</sub> ... C<sub>n</sub>. We then have in the C.M. system

$$K_i + w_A + w_B = K_f + w_1 + w_2 + \cdots w_n. \quad (2.34)$$

We can rewrite this equation as

$$K_f = K_i + Q_{if} \quad (2.35)$$

where

$$Q_{if} = w_A + w_B - (w_1 + w_2 + \cdots w_n) \quad (2.36)$$

is the change in internal energy due to the reaction. Clearly a necessary condition for the reaction to occur is that

$$K_f \geq 0. \quad (2.37)$$

Therefore:

i) If  $Q_{if} \geq 0$ , the reaction is always possible from energy considerations. (It can be prevented from occurring because of other conservation laws.) Such a reaction is called *exothermic*, since a certain amount of internal energy is converted into kinetic energy during the collision.

ii) If  $Q_{if} < 0$ , the reaction is *endothermic*. The necessary condition (2.37) then reads with the help of eq. (2.35)

$$K_i \geq K_i^t = -Q_{if}. \quad (2.38)$$

The quantity  $K_i^t$  is therefore the minimum value of  $K_i$  such that the reaction is energetically allowed. It is called the *threshold of the reaction in the C.M. system*. We note that when  $K_i = K_i^t$  all the outgoing particles have a vanishing

kinetic energy in the C.M. system ( $K_i = 0$ ). The corresponding *threshold energy*  $(K_i)_L$  in the laboratory system may easily be found by using eq. (2.13). It is given by

$$(K_i)_L = \frac{m_A + m_B}{m_B} K_i^t. \quad (2.39)$$

Clearly, at threshold all the outgoing particles have in the laboratory system a velocity  $V_L$  equal to that of the center of mass.

### 2.1.3. Relations between cross sections

Let us consider again the reaction (2.21) with two particles C and D in the final state (see Figs. 2.3 and 2.4). From the definition of the cross sections given in Section 1.3, we know that the same number of particles C are emitted into the solid angle  $d\Omega$  about the direction  $(\theta, \phi)$  as are emitted into  $d\Omega_L$  about  $(\theta_L, \phi_L)$ . Thus [see eq. (1.27)]

$$\frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) d\Omega_L = \frac{d\sigma_C}{d\Omega}(\theta, \phi) d\Omega \quad (2.40)$$

or

$$\frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) \sin \theta_L d\theta_L d\phi_L = \frac{d\sigma_C}{d\Omega}(\theta, \phi) \sin \theta d\theta d\phi. \quad (2.41)$$

From the last of eqs. (2.6) we immediately note that  $d\phi_L = d\phi$ . Moreover, we may also use eqs. (2.8) and (2.9) which we rewrite more explicitly in our case as

$$\cos \theta_L = \frac{\cos \theta + \tau_C}{(1 + 2\tau_C \cos \theta + \tau_C^2)^{1/2}} \quad (2.42)$$

with

$$\tau_C = V_L/v_C. \quad (2.43)$$

Before we proceed with eq. (2.42), let us first obtain a more useful expression of  $\tau_C$ . We first remark that since

$$(P)_L = M(V)_L = m_A(v_A)_L \quad (2.44)$$

we have

$$V_L = \frac{m_A}{m_A + m_B} (v_A)_L = \frac{(p_A)_L}{m_A + m_B} \quad (2.45)$$

or, using eqs. (2.10) and (2.13)

$$V_L = \left[ \frac{2m_A K_i}{m_B(m_A + m_B)} \right]^{1/2}. \quad (2.46)$$

We may also obtain eq. (2.46) by noting that

$$V_L = v_B = p_i/m_B \quad (2.47)$$



and then using eqs. (2.19) and (2.20) to express  $p_i$  in terms of  $K_i$ ,  $m_A$  and  $m_B$ . On the other hand, from eq. (2.28) and the fact that  $p_f = p_C = m_C v_C$ , we deduce that

$$v_C = \frac{p_f}{m_C} = \left[ \frac{2m_D K_f}{m_C(m_C + m_D)} \right]^{1/2}. \quad (2.48)$$

Hence, from eqs. (2.35), (2.43), (2.46) and (2.48), we find that

$$\tau_C = \left[ \frac{m_A m_C}{m_B m_D} \frac{K_i}{K_i + Q_{if}} \right]^{1/2} \quad (2.49)$$

where we have used the fact that the collision is non-relativistic to set the ratio  $(m_A + m_B)/(m_C + m_D)$  equal to one [6]. A similar calculation for the emission of particle D yields

$$\tau_D = \frac{V_L}{v_D} = \left[ \frac{m_A m_D}{m_B m_C} \frac{K_i}{K_i + Q_{if}} \right]^{1/2}. \quad (2.50)$$

It is important to note that only for collisions with *two* particles in the final state are the quantities  $\tau_C = V_L/v_C$  and  $\tau_D = V_L/v_D$  *fixed* at a given initial energy [8]. For these collisions we may therefore readily differentiate eq. (2.42) and obtain with the help of eq. (2.41)

$$\frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) = \frac{(1 + \tau_C^2 + 2\tau_C \cos \theta)^{3/2}}{|1 + \tau_C \cos \theta|} \frac{d\sigma_C}{d\Omega}(\theta, \phi). \quad (2.51)$$

Since in the C.M. system the two particles C and D move in opposite directions (see Fig. 2.4) it is clear that the differential cross section for observation of the particle D in the direction  $(\theta, \phi)$  is just

$$\frac{d\sigma_D}{d\Omega}(\theta, \phi) = \frac{d\sigma_C}{d\Omega}(\pi - \theta, \phi + \pi) \quad (2.52)$$

while the corresponding differential cross section for emission of the particle D in the laboratory system is given by

$$\frac{d\sigma_D}{d\Omega_L}(\theta_L, \phi_L) = \frac{(1 + \tau_D^2 + 2\tau_D \cos \theta)^{3/2}}{|1 + \tau_D \cos \theta|} \frac{d\sigma_D}{d\Omega}(\theta, \phi). \quad (2.53)$$

Finally, we recall [see eq. (1.28)] that the *total* cross section for emission of particles C (or D) is the same for both laboratory and center of mass systems.

The above formulae have been obtained in the case of a reaction (2.21) with two particles C and D in the final state. These formulae evidently simplify for elastic collisions (1.1) or inelastic processes of the type (1.2). On the contrary, the case of reactions with  $n \geq 3$  particles in the final state is more involved, since the number of kinematical variables grows rapidly with increasing  $n$  and a variety of differential cross sections may be defined, depending on the quantities which are held fixed during the experiment. We shall return to this question in Section 2.2.4 and also in Chapter 15.

## 2.2. Relativistic kinematics [9]

### 2.2.1. Preliminaries

The energy  $E$ , rest mass  $m$  and momentum  $\mathbf{p}$  of a particle are now related by

$$E = \sqrt{m^2 c^4 + \mathbf{p}^2 c^2}, \quad (2.54)$$

where  $c$  is the velocity of light. In terms of the velocity  $\mathbf{v}$  of the particle, we have

$$\mathbf{p} = m\gamma\mathbf{v} \quad (2.55)$$

and

$$E = m\gamma c^2 \quad (2.56)$$

where we have defined the quantity

$$\gamma = (1 - v^2/c^2)^{-1/2}. \quad (2.57)$$

We can also write

$$\mathbf{v} = v\hat{\mathbf{p}} \quad (2.58)$$

where

$$v = dE/dp = c^2 p/E. \quad (2.59)$$

Relativistic phenomena are described within the framework of the Minkowski space-time. An “event” or world point is specified by the set of four space-time coordinates

$$X \equiv (ct, x, y, z) \quad (2.60)$$

or

$$X \equiv (x_0, x_1, x_2, x_3) \equiv (x_0, \mathbf{X}) \quad (2.61)$$

with

$$x_0 = ct, \quad \mathbf{X} \equiv (x_1, x_2, x_3). \quad (2.62)$$

The four component object  $X$  is called a four-vector while the “ordinary” three component vector  $\mathbf{X}$  is often denoted as a three-vector. The squared norm of the four-vector  $X$  is defined [10] as

$$X^2 = x_0^2 - |\mathbf{X}|^2 = c^2 t^2 - x^2 - y^2 - z^2 \quad (2.63)$$

where we have denoted by  $|\mathbf{X}|^2$  the squared norm of the three-vector  $\mathbf{X}$ . Similarly, the lengths of the three- and four-vectors  $\mathbf{X}$  and  $X$  will be written respectively as  $|\mathbf{X}|$  and  $X$  [11].

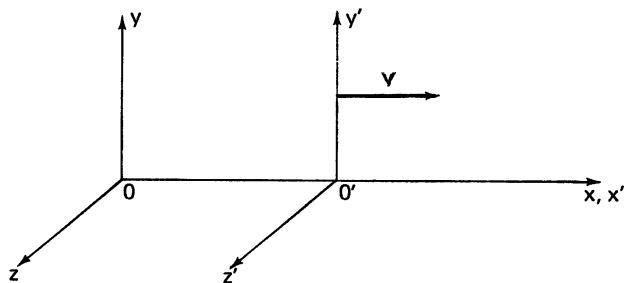


Fig. 2.5. Illustration of a special proper Lorentz transformation. The coordinate system  $(0'x'y'z')$  moves with respect to  $(0xyz)$  with a velocity  $v$  in the direction of the  $x$ -axis.

Lorentz transformations are real, linear transformations of space-time coordinates leaving invariant the quadratic form  $c^2t^2 - x^2 - y^2 - z^2$  (i.e. the distance between points in Minkowski space-time). Such transformations express the fact that the velocity of light is the same in all inertial systems (Lorentz frames). Excluding the translations in space-time [12] together with reflections in space alone, time alone, or both, we are left with *proper Lorentz transformations*. If we still disregard the rotations in ordinary space, we obtain *special proper Lorentz transformations*. An example of these is given in Fig. 2.5, where the Lorentz frame  $(0'x'y'z')$  moves with respect to  $(0xyz)$  with a velocity  $\mathbf{v} = v\hat{x}$ . Furthermore, the axes of the two systems are parallel. The corresponding special proper Lorentz transformation, also called a “boost” in the  $x$ -direction, is given by [3]

$$\begin{cases} x = \gamma(x' + \beta ct') \\ y = y' \\ z = z' \\ ct = \gamma(ct' + \beta x') \end{cases} \quad (2.64)$$

where  $\gamma$  is given by eq. (2.57) and  $\beta = v/c$ . Obviously, since the frame  $(0xyz)$  moves with respect to  $(0'x'y'z')$  with a velocity  $-\mathbf{v}$ , we have also the inverse relations

$$\begin{cases} x' = \gamma(x - \beta ct) \\ y' = y \\ z' = z \\ ct' = \gamma(ct - \beta x) \end{cases} \quad (2.65)$$

The general proper Lorentz transformation may be obtained by combining a number of special proper Lorentz transformations and ordinary rotations about the  $x$ ,  $y$  and  $z$  axis. All quantities which consist of a set of four numbers transforming under a Lorentz transformation as the components of  $X \equiv (ct, x, y, z)$  are called four-vectors. Since the squared norm (2.63) of  $X$  is an invariant under Lorentz transformations, and because any four-vector  $a \equiv (a_0, a_x, a_y, a_z)$  transforms like  $X$ , the squared norm of  $a$ , namely

$$a^2 = a_0^2 - a_x^2 - a_y^2 - a_z^2 \quad (2.66)$$

must also be an invariant. Furthermore, if  $a$  and  $b$  are four-vectors, so is their sum  $(a + b)$ . Thus the quantity  $(a + b)^2 = a^2 + 2ab + b^2$  is an invariant and therefore also the scalar product

$$ab = a_0b_0 - \mathbf{a} \cdot \mathbf{b} = a_0b_0 - a_xb_x - a_yb_y - a_zb_z. \quad (2.67)$$

Four-vectors such that  $a^2 < 0$  are called space-like. Those with  $a^2 > 0$  are time-like, while those with  $a^2 = 0$  are null vectors. This classification corresponds to the position of the four-vector with respect to the light cone

$$c^2t^2 - x^2 - y^2 - z^2 = 0. \quad (2.68)$$

Of particular importance is the time-like energy-momentum four-vector (or four-momentum)  $p \equiv (E/c, \mathbf{p})$  such that, according to eq. (2.54)

$$p^2 = E^2/c^2 - |\mathbf{p}|^2 = m^2 c^2. \quad (2.69)$$

In what follows, and in order to simplify the formulae, we shall frequently choose units such that  $c = 1$ .

### 2.2.2. Laboratory and center of mass systems

Let us consider a relativistic collision between the two particles A and B. We still define the *laboratory system* as that coordinate system where particle B is at rest before the collision. In the laboratory system the four-momenta of particles A and B are respectively  $(p_A)_L \equiv ((E_A)_L, (\mathbf{p}_A)_L)$  and  $(p_B)_L \equiv (m_B, \mathbf{0})$ . The *center of mass, center of momentum (C.M.)* or *barycentric system* is the coordinate system for which

$$\mathbf{p}_A + \mathbf{p}_B = \mathbf{0} \quad (2.70)$$

where  $p_A \equiv (E_A, \mathbf{p}_A)$  and  $p_B \equiv (E_B, \mathbf{p}_B)$  denote the four-momenta of particles A and B in the C.M. system. The laboratory and C.M. systems are therefore two particular Lorentz frames, such that the velocity of the C.M. system in the laboratory system is  $\mathbf{V}_L$ . Let us choose the incident direction as the  $z$ -axis in both coordinate systems, so that in the laboratory system

$$\mathbf{V}_L = V_L \hat{z} \quad (2.71)$$

and let the directions of the axes of the two frames be parallel (see Fig. 2.6). Then the Lorentz transformation from the C.M. system to the laboratory system is a special proper Lorentz transformation, namely a "boost" in the  $z$ -direction. Comparing Figs. 2.5 and 2.6 and using eqs. (2.64) we see that (with  $c = 1$ )

$$\begin{cases} x_L = x \\ y_L = y \\ z_L = \gamma(z + V_L t) \\ t_L = \gamma(t + V_L z) \end{cases} \quad (2.72)$$

with now

$$\gamma = (1 - V_L^2)^{-1/2}. \quad (2.73)$$

Clearly, since the laboratory system moves with velocity  $-\mathbf{V}_L$  as seen in the C.M. system, we also have

$$\begin{cases} x = x_L \\ y = y_L \\ z = \gamma(z_L - V_L t_L) \\ t = \gamma(t_L - V_L z_L). \end{cases} \quad (2.74)$$

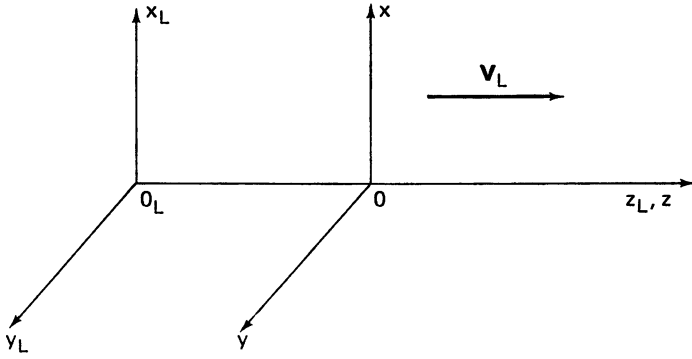


Fig. 2.6. The two Lorentz frames  $(0_Lx_Ly_Lz_L)$  and  $(0xyz)$  of the text. The C.M. system  $(0xyz)$  moves with respect to the laboratory system  $(0_Lx_Ly_Lz_L)$  with constant velocity  $V_L = V_L\hat{z}$ .

We have already noted above that the four-momentum  $p \equiv (E, \mathbf{p})$  transforms as the coordinates  $X \equiv (x_0, \mathbf{X})$ . Therefore, using eqs. (2.72) we see that

$$\begin{cases} (p_x)_L = p_x \\ (p_y)_L = p_y \\ (p_z)_L = \gamma(p_z + V_L E) \\ E_L = \gamma(E + V_L p_z). \end{cases} \quad (2.75)$$

How do the velocities transform? Let us call  $\mathbf{v}$  the velocity of a particle in the C.M. system and  $\mathbf{v}_L$  its velocity in the laboratory system. We assume that the velocities  $\mathbf{v}$  and  $\mathbf{v}_L$  make angles  $\theta$  and  $\theta_L$ , respectively, with the  $z$ -axis (see

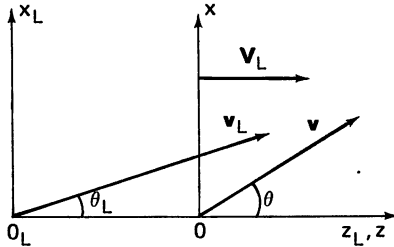


Fig. 2.7. Illustration of the velocities  $\mathbf{v}_L$  and  $\mathbf{v}$  of the text.

Fig. 2.7). Furthermore, we choose the coordinate axes so that  $\mathbf{v}$  lies in the  $(xz)$  and  $(x_Lz_L)$  planes. Then, by differentiating eqs. (2.72) we obtain

$$(v_z)_L = v_L \cos \theta_L = \frac{v \cos \theta + V_L}{1 + V_L v \cos \theta / c^2} \quad (2.76)$$

and

$$(v_x)_L = v_L \sin \theta_L = \frac{v \sin \theta}{1 + V_L v \cos \theta / c^2} \quad (2.77)$$

where we have written explicitly the velocity of light  $c$  and used the fact that  $\gamma = (1 - V_L^2/c^2)^{-1/2}$ . If the two velocities  $v$  and  $V_L$  are parallel, then

$$v_L = \frac{v + V_L}{1 + V_L v/c^2}. \quad (2.78)$$

We note that eqs. (2.76)–(2.78) reduce to the simple Galilean results (2.5)–(2.6) when both  $v/c \ll 1$  and  $V_L/c \ll 1$ . From eqs. (2.76) and (2.77) we also find that

$$\tan \theta_L = \frac{1}{\gamma} \frac{\sin \theta}{\cos \theta + \tau} \quad (2.79)$$

where

$$\tau = V_L/v \quad (2.80)$$

so that eq. (2.79) gives the transformation of scattering angles from the C.M. to the laboratory system. We note that this formula correctly reduces to eq. (2.7) in the non-relativistic limit.

How is the velocity  $V_L$  related to the momenta and energies of the particles participating in the collision? For a channel containing  $n$  particles, we can use eqs. (2.75) to write the  $z$ -component of the total momentum in the laboratory system as

$$(P_z)_L = \gamma V_L E \quad (2.81)$$

where  $E$  is the total energy in the C.M. system. In obtaining eq. (2.81) we have used the fact that  $\mathbf{P} = 0$  in the C.M. system. From eqs. (2.75) we can also write the total laboratory energy as

$$E_L = \gamma E \quad (2.82)$$

so that

$$V_L = \frac{(P_z)_L}{E_L} = \frac{\sum_{j=1}^n |\mathbf{p}_j|_L \cos(\theta_j)_L}{\sum_{j=1}^n (E_j)_L} \quad (2.83)$$

where  $(\theta_j)_L$  is the angle between the vector  $(\mathbf{p}_j)_L$  and the  $z$ -axis in the laboratory system. In particular, for the initial channel (A + B)

$$V_L = \frac{|\mathbf{p}_A|_L}{(E_A)_L + m_B} \quad (2.84)$$

Since the norm of a four-vector is a Lorentz-invariant, the total C.M. energy  $E = E_A + E_B$  is also a Lorentz-invariant. This follows from the fact that the invariant quantity  $s = (p_A + p_B)^2$  may be written as

$$s = (p_A + p_B)^2 = (E_A + E_B)^2 - (\mathbf{p}_A + \mathbf{p}_B)^2 = (E_A + E_B)^2 \quad (2.85)$$

since  $\mathbf{p}_A + \mathbf{p}_B = 0$  in the C.M. system. The same quantity  $s$  evaluated in the laboratory system is given by

$$\begin{aligned} s &= [(E_A)_L + m_B]^2 - (\mathbf{p}_A)_L^2 \\ &= (E_A)_L^2 + 2m_B(E_A)_L + m_B^2 - (\mathbf{p}_A)_L^2. \end{aligned} \quad (2.86)$$

But

$$(E_A)_L^2 - (p_A)_L^2 = m_A^2$$

and therefore

$$s = m_A^2 + m_B^2 + 2m_B(E_A)_L. \quad (2.87)$$

Introducing the kinetic energy of the incident particle in the laboratory system

$$(K_A)_L = (E_A)_L - m_A \quad (2.88)$$

we also have

$$s = (m_A + m_B)^2 + 2m_B(K_A)_L. \quad (2.89)$$

At very high energies, where

$$|p_A|_L \gg m_A, m_B \quad (2.90)$$

and

$$(E_A)_L \simeq |p_A|_L \quad (2.91)$$

we note that eq. (2.87) becomes

$$s \simeq 2m_B |p_A|_L \quad (2.92)$$

so that the square of the C.M. *energy* grows linearly with the laboratory incident *momentum* at ultra-relativistic energies.

As a first application of these formulae, let us consider a colliding beam experiment in which two protons, of mass  $m_p \simeq 0.94$  GeV, move towards each other with C.M. three-momenta of magnitude  $|p_A| = |p_B| = 30$  GeV/ $c$ . Thus

$$E_A = E_B = \sqrt{0.88 + 900} \text{ GeV} \simeq 30 \text{ GeV}$$

and the invariant quantity  $s$  is given by

$$s = (E_A + E_B)^2 \simeq 3600 \text{ GeV}^2.$$

According to eq. (2.92), we see that the same value of  $s$  would require a laboratory [13] three-momentum of magnitude

$$|p_A|_L \simeq s/2m_p \simeq 1900 \text{ GeV}/c.$$

This clearly shows the interest of using colliding beam experiments to explore the domain of such high-energy collisions.

As another example, let us calculate the value of  $(E_A)_L$  at the threshold of a reaction

$$A + B \rightarrow C_1 + C_2 + \cdots + C_n \quad (2.93)$$

with  $n$  particles of masses  $m_i$  ( $i = 1, 2, \dots, n$ ) in the final state. At threshold, all outgoing particles have no momentum in the C.M. system, so that

$$s = m_A^2 + m_B^2 + 2m_B(E_A)_L = \left( \sum_{i=1}^n m_i \right)^2$$

where  $(E_A)_L$  is the threshold value of  $(E_A)_L$ . Thus,

$$(E_A)_L = \frac{1}{2m_B} \left[ \left( \sum_{i=1}^n m_i \right)^2 - m_A^2 - m_B^2 \right]. \quad (2.94)$$

A similar calculation for the threshold value of the kinetic energy  $(K_A)_L$  yields

$$(K_A)_L = -Q_{\text{if}} \frac{m_A + m_B + \sum_{i=1}^n m_i}{2m_B} \quad (2.95)$$

where

$$Q_{\text{if}} = m_A + m_B - \sum_{i=1}^n m_i \quad (2.96)$$

is the relativistic equivalent of the change of internal energy ("reaction heat") defined in eq. (2.36).

We may also evaluate the magnitude of the initial relative three-momentum vector  $\mathbf{p}_i$  in the C.M. system in terms of invariants. Defining as in eq. (2.17)

$$\mathbf{p}_i = \mathbf{p}_A = -\mathbf{p}_B \quad (2.97)$$

we have

$$s = (E_A + E_B)^2 = (\sqrt{m_A^2 + \mathbf{p}_i^2} + \sqrt{m_B^2 + \mathbf{p}_i^2})^2 \quad (2.98)$$

so that

$$|\mathbf{p}_i| = \frac{1}{2\sqrt{s}} \sqrt{(s - m_A^2 - m_B^2)^2 - 4m_A^2 m_B^2}. \quad (2.99)$$

Introducing the "triangle function" [e.g. 14, 15]

$$\lambda(x, y, z) = (x - y - z)^2 - 4yz = x^2 + y^2 + z^2 - 2xy - 2yz - 2zx, \quad (2.100)$$

which is symmetric in all its arguments, we have

$$|\mathbf{p}_i| = \frac{1}{2\sqrt{s}} \sqrt{\lambda(s, m_A^2, m_B^2)}. \quad (2.101)$$

From eq. (2.101) we obtain at once

$$E_A = \sqrt{m_A^2 + |\mathbf{p}_i|^2} = \frac{1}{2\sqrt{s}} (s + m_A^2 - m_B^2) \quad (2.102)$$

and

$$E_B = \sqrt{m_B^2 + |\mathbf{p}_i|^2} = \frac{1}{2\sqrt{s}} (s - m_A^2 + m_B^2). \quad (2.103)$$

To conclude this section we shall discuss the transformation of differential cross sections from one Lorentz frame to another. For collisions with *two* particles C and D in the final state we may follow a method similar to that used in Section 2.1.3 in the non-relativistic case. Indeed, from eq. (2.79) and the fact that the quantity  $\tau_C = V_L/v_C$  does not depend on  $\theta$  (since there are only two particles in the final channel), we may write

$$\frac{d\sigma_C}{d\Omega_L}(\theta_L, \phi_L) = \frac{[\gamma^2(\cos \theta + \tau_C)^2 + \sin^2 \theta]^{3/2}}{\gamma|1 + \tau_C \cos \theta|} \frac{d\sigma_C}{d\Omega}(\theta, \phi) \quad (2.104)$$



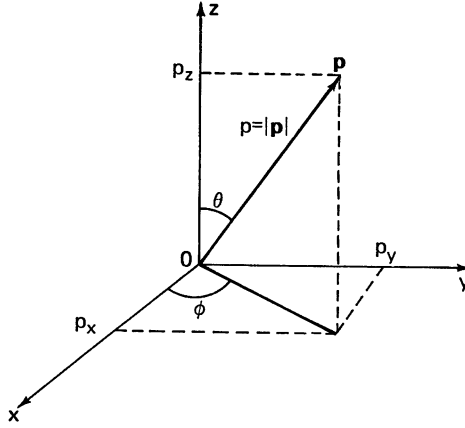


Fig. 2.8. Illustration of the spherical polar coordinates  $(p, \theta, \phi)$  of the text.

with  $\gamma = (1 - V_L^2/c^2)^{-1/2}$ . A similar formula relates the C.M. and laboratory differential cross sections corresponding to the emission of the particle D, with  $\tau_C$  replaced by  $\tau_D = V_L/v_D$ .

A more general way of looking at the transformation of differential cross sections from one Lorentz frame to the other may be devised as follows [16]. Let us suppose that the cross section of a given kind of particles is expressed in both systems in terms of solid angle and momentum. In this case the number of particles of that kind going into the solid angle element  $d\Omega$  and having a momentum between  $p$  and  $p + dp$  in the first Lorentz frame must be the same as the number of these particles going into the corresponding solid angle  $d\Omega'$  with a corresponding momentum between  $p'$  and  $p' + dp'$  in the other Lorentz frame. Thus

$$\frac{\partial^2 \sigma(p, \Omega)}{\partial p \partial \Omega} dp d\Omega = \frac{\partial^2 \sigma'(p', \Omega')}{\partial p' \partial \Omega'} dp' d\Omega' \quad (2.105)$$

with  $d\Omega = \sin \theta d\theta d\phi$  and  $d\Omega' = \sin \theta' d\theta' d\phi'$ . A simple calculation, using the special proper Lorentz transformation along the z-axis

$$\begin{cases} p_x = p'_x \\ p_y = p'_y \\ p_z = \gamma(p'_z + \beta E') \\ E = \gamma(E' + \beta p'_z) \end{cases} \quad (2.106)$$

together with the relations defining the spherical polar coordinates  $(p, \theta, \phi)$  and  $(p', \theta', \phi')$ , namely (see Fig. 2.8)

$$\begin{cases} p_x = p \sin \theta \cos \phi \\ p_y = p \sin \theta \sin \phi \\ p_z = p \cos \theta \end{cases} \quad \begin{cases} p'_x = p' \sin \theta' \cos \phi' \\ p'_y = p' \sin \theta' \sin \phi' \\ p'_z = p' \cos \theta' \end{cases} \quad (2.107)$$

yields the Jacobian

$$\frac{\partial(p\Omega)}{\partial(p'\Omega')} = \frac{E \sin^2 \theta}{E' \sin^2 \theta'} = \frac{p'^2 E}{p^2 E'}. \quad (2.108)$$

Therefore

$$\frac{\partial^2 \sigma(p, \Omega)}{\partial p \partial \Omega} = \frac{\partial^2 \sigma'(p', \Omega')}{\partial p' \partial \Omega'} \frac{E' \sin^2 \theta'}{E \sin^2 \theta}. \quad (2.109)$$

Similarly, if the differential cross sections are expressed in both Lorentz frames in terms of solid angle and energy, one finds that

$$\frac{\partial^2 \sigma(E, \Omega)}{\partial E \partial \Omega} = \frac{\partial^2 \sigma'(E', \Omega')}{\partial E' \partial \Omega'} \frac{\sin \theta'}{\sin \theta}. \quad (2.110)$$

### 2.2.3. Collisions with two particles in the final state

We now concentrate on the relativistic kinematics of two-body reactions

$$A + B \rightarrow C + D. \quad (2.111)$$

We denote respectively by  $m_A$ ,  $m_B$ ,  $m_C$  and  $m_D$  the rest masses of the particles A, B, C and D, while their four-momenta are called  $P_A$ ,  $P_B$ ,  $P_C$  and  $P_D$ . Capital letters are used here to emphasize that these four-momenta are not necessarily evaluated in the C.M. or laboratory systems. When we wish to indicate that the four-momentum of particle A is evaluated in the C.M. system we shall use the symbol  $p_A$  as in the previous sections. Similarly, the corresponding laboratory four-momentum will be called  $(p_A)_L$ .

Conservation of energy and momentum gives

$$P_A + P_B = P_C + P_D \quad (2.112)$$

with the additional constraints [see eq. (2.69)]

$$P_A^2 = m_A^2, \quad P_B^2 = m_B^2, \quad P_C^2 = m_C^2, \quad P_D^2 = m_D^2 \quad (2.113)$$

which are called “mass-shell conditions”. It is convenient to introduce the three Lorentz invariant Mandelstam variables [1]

$$s = (P_A + P_B)^2 = (P_C + P_D)^2, \quad (2.114)$$

$$t = (P_A - P_C)^2 = (P_B - P_D)^2 \quad (2.115)$$

and

$$u = (P_A - P_D)^2 = (P_C - P_B)^2. \quad (2.116)$$

We now observe that one can only form *six* independent invariants with the three independent four-vectors  $P_A$ ,  $P_B$  and  $P_C$  (or  $P_D$ ). Moreover, since the four constraints (2.113) must be obeyed, the three Mandelstam variables  $s$ ,  $t$  and  $u$  are not independent. Indeed, one directly obtains from eqs. (2.114)–(2.116) the following linear relation between  $s$ ,  $t$  and  $u$ :

$$s + t + u = m_A^2 + m_B^2 + m_C^2 + m_D^2. \quad (2.117)$$

What is the physical interpretation of the Mandelstam variables? We have already seen that the quantity  $s$  is the square of the total energy in the C.M. system. Eqs. (2.115) and (2.116) show that  $t$  and  $u$  are squares of four-momentum transfers. From eq. (2.115) we have

$$t = m_A^2 + m_C^2 - 2P_A P_C = m_B^2 + m_D^2 - 2P_B P_D. \quad (2.118)$$

Next, working in the C.M. system, and using the initial and final relative three-momenta

$$\mathbf{p}_i = \mathbf{p}_A = -\mathbf{p}_B$$

and

$$\mathbf{p}_f = \mathbf{p}_C = -\mathbf{p}_D$$

we have (see Fig. 2.4)

$$t = m_A^2 + m_C^2 - 2E_A E_C + 2|\mathbf{p}_i| |\mathbf{p}_f| \cos \theta = m_B^2 + m_D^2 - 2E_B E_D + 2|\mathbf{p}_i| |\mathbf{p}_f| \cos \theta \quad (2.119)$$

where  $|\mathbf{p}_i|$  is given by eq. (2.101) and

$$|\mathbf{p}_f| = \frac{1}{2\sqrt{s}} \sqrt{\lambda(s, m_C^2, m_D^2)}. \quad (2.120)$$

Similarly, we deduce from eq. (2.116) that

$$u = m_A^2 + m_D^2 - 2E_A E_D - 2|\mathbf{p}_i| |\mathbf{p}_f| \cos \theta = m_B^2 + m_C^2 - 2E_B E_C - 2|\mathbf{p}_i| |\mathbf{p}_f| \cos \theta. \quad (2.121)$$

Using eqs. (2.119) and (2.121), we can express  $\cos \theta$  in terms of the Mandelstam variables as

$$\cos \theta = \frac{1}{\sqrt{\lambda(s, m_A^2, m_B^2) \lambda(s, m_C^2, m_D^2)}} \{s(t - u) + (m_A^2 - m_B^2)(m_C^2 - m_D^2)\}. \quad (2.122)$$

We note that for an elastic collision, where

$$m_A = m_C, \quad m_B = m_D, \quad |\mathbf{p}_i| = |\mathbf{p}_f| = |\mathbf{p}|$$

we simply have

$$t = -2|\mathbf{p}|^2(1 - \cos \theta) = -4|\mathbf{p}|^2 \sin^2 \frac{1}{2} \theta \quad (2.123)$$

while

$$u = -4|\mathbf{p}|^2 \cos^2 \frac{1}{2} \theta. \quad (2.124)$$

Other useful relations may be obtained by evaluating the quantities  $t$  and  $u$  in the laboratory system. For example, we see from eq. (2.118) that

$$t = m_B^2 + m_D^2 - 2m_B(E_D)_L = (m_B - m_D)^2 - 2m_B(K_D)_L \quad (2.125)$$

where  $(K_D)_L = (E_D)_L - m_D$  is the kinetic energy of the particle D in the laboratory system.

Apart from the fact that the Mandelstam variables are very convenient to transform kinematical quantities between the C.M. and the laboratory system, they also allow a symmetric description of the reactions

$$A + B \rightarrow C + D, \quad (2.126)$$

$$A + \bar{C} \rightarrow \bar{B} + D \quad (2.127)$$

and

$$A + \bar{D} \rightarrow \bar{B} + C \quad (2.128)$$

linked by *crossing symmetry* [e.g. 17]. Here  $\bar{B}$  is the antiparticle of  $B$ , etc. A loose way of formulating the crossing assumption is that the transition amplitude for a process containing a *particle* of four-momentum  $p$  in the initial (final) channel is identical with the transition amplitude for the “crossed” reaction containing the corresponding *antiparticle* of four-momentum  $-p$  in the final (initial) channel. Thus the Mandelstam variable  $t$ , defined by eq. (2.115) for the process (2.111) [or (2.126)] becomes

$$t = (P_A - P_C)^2 \rightarrow (P_A + P_C)^2 \quad (2.129)$$

for the crossed process (2.127). It now has the meaning of the square of the total energy for the reaction (2.127), which is called therefore the “ $t$  channel”. The original process (2.126), where the Mandelstam variable  $s$  defined by eq. (2.114) corresponds to the square of the total C.M. energy is called the “ $s$  channel”. Similarly, the process (2.128) is the “ $u$  channel” because, on invoking our crossing arguments

$$u = (P_A - P_D)^2 \rightarrow (P_A + P_D)^2. \quad (2.130)$$

As an example, let us consider the case of nucleon–nucleon scattering, neglecting the mass differences between neutron and proton. Choosing as our “ $s$  channel” the reaction

$$n + p \rightarrow n + p \quad \text{“}s\text{ channel”}, \quad (2.131)$$

we then have

$$n + \bar{n} \rightarrow p + \bar{p} \quad \text{“}t\text{ channel”} \quad (2.132)$$

and

$$n + \bar{p} \rightarrow n + \bar{p} \quad \text{“}u\text{ channel”}. \quad (2.133)$$

In the physical region of the “ $s$  channel” reaction (i.e. that domain of the variables  $s, t, u$  where the reaction (2.131) can occur) we have

$$s = 4(m^2 + |\mathbf{p}|^2) \geq 4m^2,$$

while

$$t = -4|\mathbf{p}|^2 \sin^2 \frac{1}{2}\theta \leq 0$$

and

$$u = -4|\mathbf{p}|^2 \cos^2 \frac{1}{2}\theta \leq 0.$$

Similarly, in the physical region of the “ $t$  channel” reaction we have  $t \geq 4m^2$  while  $s, u \leq 0$ . Finally, in the physical region of the “ $u$  channel” reaction, one has  $u \geq 4m^2$  and  $s, t \leq 0$ .

This situation can be clearly illustrated by using a diagram suggested by Mandelstam [1], which describes the variables  $s$ ,  $t$  and  $u$  in a symmetric way on a two-dimensional plot. The Mandelstam diagram for the symmetric case considered here is illustrated in Fig. 2.9.

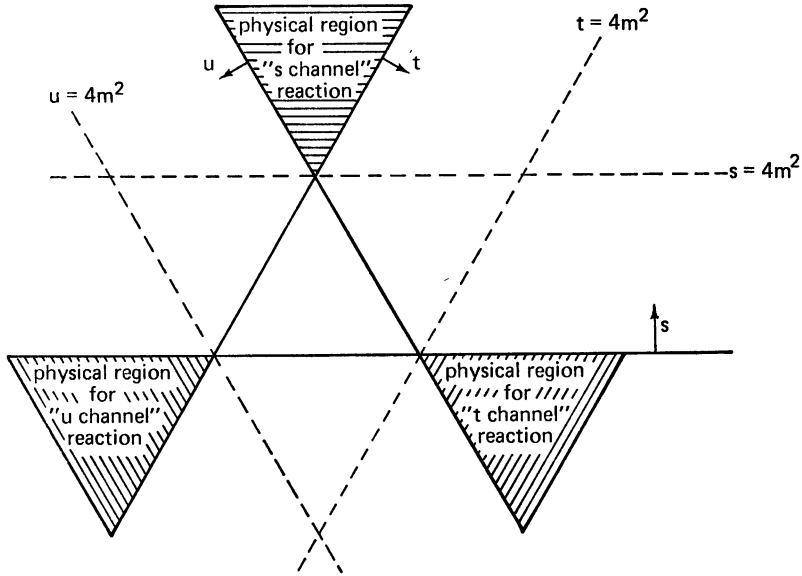


Fig. 2.9. The Mandelstam diagram for equal mass elastic scattering.

This analysis has been extended by Kibble [18] to the case of four arbitrary masses, with the following results. The physical regions corresponding to the three processes (2.126)–(2.128) do not overlap and are delimited by the three branches of a cubic curve. (In the equal mass case the cubic “degenerates” into three straight lines). In general, there exists also a central loop in any Mandelstam diagram (for example the central triangle in Fig. 2.9). This loop corresponds to the physical region of the decay process

$$A \rightarrow \bar{B} + C + D \quad (2.134)$$

provided this process is energetically possible, i.e. if

$$m_A > m_B + m_C + m_D. \quad (2.135)$$

#### 2.2.4. Collisions with three and more particles in the final state

We now consider relativistic collisions of the type

$$A + B \rightarrow C_1 + C_2 + \cdots C_n. \quad (2.136)$$

For such a reaction one can form  $3n - 4$  independent Lorentz-invariant variables [19]. We define again

$$s = (P_A + P_B)^2 = (P_1 + P_2 + \cdots P_n)^2 \equiv P^2. \quad (2.137)$$

We may also consider the quantities

$$s_{ij} = (P_i + P_j)^2 = m_i^2 + m_j^2 + 2E_i E_j - 2|P_i| |P_j| \cos \theta_{ij} \quad (i, j = 1, 2, \dots, n) \quad (2.138)$$

where  $\theta_{ij}$  is the angle between the three-vectors  $P_i$  and  $P_j$ . The *effective mass* of particles  $i$  and  $j$  is defined as the square root of  $s_{ij}$ . A separate C.M. system for particles  $i$  and  $j$  can be defined by requiring that

$$P_i + P_j = 0 \quad (2.139)$$

so that, in this frame, the effective mass of particles  $i$  and  $j$  is simply

$$\sqrt{s_{ij}} = E_i + E_j. \quad (2.140)$$

This frame is particularly convenient to discuss the decay process

$$X \rightarrow C_i + C_j \quad (2.141)$$

because it coincides with the rest frame of the unstable particle  $X$ .

We may extend the concept of effective mass to an arbitrary number of particles. For example, the quantity

$$s_{ijk} = (P_i + P_j + P_k)^2 = s_{ij} + s_{jk} + s_{ik} - m_i^2 - m_j^2 - m_k^2 \quad (2.142)$$

is the square of the effective mass of particles  $i, j$  and  $k$ . If there are only three particles in the final state, we have,

$$s_{12} = (P_1 + P_2)^2 = (P - P_3)^2 = s + m_3^2 - 2E_3 \sqrt{s} \quad (2.143)$$

where  $E_3$  is the energy of particle 3 in the (over-all) C.M. system and we have used the fact that  $P = 0$  in that frame. We see from eq. (2.143) that the C.M. energy of one of the three particles is determined by the total C.M. energy together with the effective mass of the two other particles.

Finally, we can also introduce the  $2n$  four-momentum transfers

$$t_{Ai} = (P_A - P_i)^2, \quad i = 1, 2, \dots, n \quad (2.144)$$

and

$$t_{Bi} = (P_B - P_i)^2, \quad i = 1, 2, \dots, n. \quad (2.145)$$

Since there are only  $3n - 4$  independent Lorentz-invariant variables, the effective masses and four-momentum transfers defined above are not all independent. The best choice of variables often depends on the particular process being considered. In fact, although the effective masses and four-momentum transfers defined above are obvious candidates to describe multiparticle reactions of the type (2.136), it is sometimes convenient to introduce other kinematical variables [e.g. 20, 21].

There exists also a variety of ways to "represent" processes of the type (2.136) on two-dimensional diagrams. For example, in the case of a reaction

$$A + B \rightarrow C_1 + C_2 + C_3 \quad (2.146)$$

or a decay

$$X \rightarrow C_1 + C_2 + C_3 \quad (2.147)$$

each “event” can be plotted as a point in the  $(E_1, E_2)$  plane or equivalently [see eq. (2.143)] as a point in the  $(s_{23}, s_{13})$  plane. This is called a *Dalitz plot* [22], an example of which is given in Fig. 2.10. Another important diagram

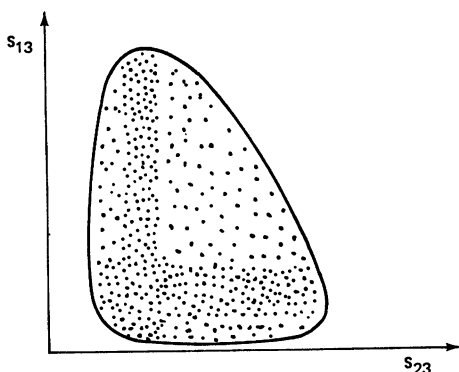


Fig. 2.10. Dalitz plot for a production process  $A + B \rightarrow C_1 + C_2 + C_3$ . Dots indicate observed events.

for the production process (2.146) is the Chew–Low plot [23], where events are plotted in the  $(t_{A3}, s_{12})$  plane. In the case of four particles in the final state, a frequently used diagram is the *scatter plot*, such that events are recorded in the plane  $(s_{12}, s_{34})$ .

## References and notes

- [1] MANDELSTAM, S. (1958), *Phys. Rev.* **112**, 1344.
- [2] BALDIN, A. M., V. I. GOLDANSKY and I. L. ROSENAL (1961), *Kinematics of Nuclear Reactions*, translated from Russian (Pergamon Press).
- [3] HAGEDORN, R. (1963), *Relativistic Kinematics* (Benjamin, New York).
- [4] MICHALOWICZ, A. (1964), *Cinématique des Réactions Nucléaires* (Dunod, Paris).
- [5] It is worth pointing out that the use of these geometrical relationships is valid in the kinematical study of *quantum* as well as *classical collisions*. Indeed such geometrical relations are applied essentially to momentum vectors in the asymptotic region where the particles need not be precisely localized in space. These particles can therefore have a well defined momentum in the asymptotic region without violating the Heisenberg uncertainty principle.
- [6] Since the collision is non-relativistic we may write here  $M = m_A + m_B = m_C + m_D$ .
- [7] The internal energy of a (composite) particle is here defined as the binding energy of that system. For example, if the particle A is an hydrogen atom in its ground state the corresponding internal energy is  $w_A = -1$  Rydberg  $\simeq -13.6$  eV.
- [8] Note also that the corresponding laboratory quantities  $(\tau_c)_L = V_L/(v_c)_L$  and  $(\tau_D)_L = V_L/(v_D)_L$  are not fixed for a given initial energy since  $(v_c)_L$  and  $(v_D)_L$  depend on the angle  $\theta_L$ .
- [9] This section is of a higher level of difficulty and may be studied after Part II, which is entirely devoted to non-relativistic scattering.

- [10] Another convention consists in defining  $x_1 = x$ ,  $x_2 = y$ ,  $x_3 = z$ ,  $x_4 = ict$ , with  $X^2 = \sum_{\mu=1}^4 x_{\mu}x_{\mu} = x^2 + y^2 + z^2 - c^2t^2$ .
- [11] These conventions will only be used when there is a possibility of confusion between three- and four-vectors. In cases where no such ambiguity may arise, we shall continue to denote by  $X^2$  or  $\mathbf{X}^2$  the squared norm of an ordinary three-vector  $\mathbf{X}$  and by  $X$  its length. We also remark that the conventions used here imply that the *length*  $X = |\mathbf{X}|$  of a vector  $\mathbf{X}$  is identical to its *norm*, which is often denoted by the symbol  $||\mathbf{X}||$ .
- [12] Lorentz transformations including translations in space-time are called inhomogeneous Lorentz transformations (or Poincaré transformations).
- [13] Remember that the laboratory system is the reference frame in which the target (not the experimentalist!) is at rest. In the present example the "target" is any one of the two colliding protons and the observer is actually at rest in the C.M. system.
- [14] KÄLLEN, G. (1964), *Elementary Particle Physics* (Addison-Wesley, Reading, Mass.) Chapter 1.
- [15] PILKUHN, H. (1967), *The Interaction of Hadrons* (North-Holland, Amsterdam) Chapter 1.
- [16] More details about this method may be found in ref. [3], Chapter 5.
- [17] OMNÈS, R. and M. FROISSART (1963), *Mandelstam Theory and Regge Poles* (Benjamin, New York) Chapter 5.
- [18] KIBBLE, T. W. (1960), Phys. Rev. **117**, 1159.
- [19] Note that in the particular case  $n = 2$  we have shown indeed that there are  $3n - 4 = 2$  independent Lorentz invariant variables, for example  $s$  and  $t$ .
- [20] BALI, N., G. F. CHEW and A. PIGNOTTI (1967), Phys. Rev. **163**, 1572.
- [21] VAN HOVE, L. (1971), Physics Reports **1C**, 347.
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# Problems to Part I

1. A thin foil of gold of surface density  $9.2 \times 10^{-4} \text{ g/cm}^2$  is bombarded by electrons of 150 MeV energy coming from a linear accelerator. The accelerator produces pulses at a rate of 60 per second and each pulse contains  $10^9$  electrons. After focusing, the cross sectional area of the incident beam is  $3 \text{ mm}^2$ .
  - a) Compute the incident electron flux  $\Phi_A$  and the average number  $\mathcal{N}_A$  of electrons per  $\text{cm}^3$  in the incident beam.
  - b) Assume that a (100% efficient) detector of surface area  $20 \text{ cm}^2$ , placed at 50 cm of the target, and at a laboratory angle of  $50^\circ$  has detected on the average 1.3 elastically scattered electrons per second. What is the corresponding elastic differential cross section? [Note: the atomic mass of gold is 197 a.m.u. and Avogadro's number is  $N_0 = 6.02 \times 10^{23}$ .]
2. Consider the scattering of  $K^+$  mesons of momentum  $2 \text{ GeV}/c$ , incident on protons. These are contained in a bubble chamber target of length 1 m, filled with liquid hydrogen (whose density is  $0.071 \text{ g/cm}^3$ ). The average number of interactions per cm path for a  $K^+$  meson is measured to be 0.08. What is the corresponding total cross section?
3. Show that in a non-relativistic two-body collision the kinetic energy  $K_L$  of a particle in the laboratory system is related to its kinetic energy  $K$  in the center of mass system by the relation

$$K_L = K(1 + \tau^2 + 2\tau \cos \theta)$$

where  $\tau$  is given by eq. (2.9) and  $\theta$  is the angle between the center of mass velocity  $\mathbf{v}$  of the particle and the incident direction.

4. Let  $(K_i)_L = (K_A)_L$  be the initial kinetic energy in the laboratory system of a non-relativistic binary reaction  $A + B \rightarrow C + D$ . Prove that the center of mass kinetic energies of the two outgoing particles C and D are given respectively by

$$K_C = \frac{m_D(K_i + Q_{if})}{m_C + m_D}, \quad K_D = \frac{m_C(K_i + Q_{if})}{m_C + m_D}$$

where  $K_i = m_B(K_i)_L/(m_A + m_B)$  is the initial kinetic energy available in the C.M. system and  $Q_{if}$  is the change of internal energy occurring in the reaction. Find the corresponding laboratory energies  $(K_C)_L$  and  $(K_D)_L$ .

5. Consider a non-relativistic elastic scattering collision between two particles A and B, of masses  $m_A$  and  $m_B$ .

a) Obtain the laboratory scattering angles of the two outgoing particles in terms of their respective center of mass scattering angles. Show in particular that in the laboratory system the "target" particles B always recoil in the forward hemisphere.

b) Calculate the ratios  $(d\sigma/d\Omega_L)/(d\sigma/d\Omega)$  for both outgoing particles.

6. Use the results of the preceding problem to analyze the kinematics of low-energy neutron-proton scattering. Neglecting the mass difference between the proton and the neutron, find the ratio of the differential cross sections in the laboratory and center of mass systems. Assuming that the angular distribution is isotropic in the center of mass system, plot the quantity  $d\sigma/d\Omega_L$ .

7. Consider a merging beam experiment in which two beams containing particles of equal mass  $M$  travel along a common axis with different (non-relativistic) velocities. Calling  $\Delta K$  the energy difference of the two beams while  $v_1$  and  $v_2$  are their respective velocities in a coordinate system (S) where the observer is at rest, show that the center of mass kinetic energy  $K$  is given by

$$K = (\Delta K)^2/8\bar{K}$$

where  $\bar{K} = M\bar{v}^2/2$ , with  $\bar{v} = (v_1 + v_2)/2$ .

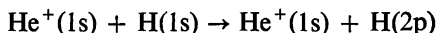
8. Assume that a proton is scattered elastically by a deuteron, the incident laboratory energy of the proton being  $(K_i)_L = 10$  MeV.

a) Obtain the center of mass velocities and kinetic energies of the proton and deuteron after the collision.

b) Find the laboratory kinetic energy of an outgoing proton scattered at an angle  $\theta = 60^\circ$  in the center of mass system. What is the laboratory kinetic energy of a deuteron recoiling at a laboratory angle  $\theta_L = 30^\circ$ ?

9. A beam of protons is incident on a gas of deuterium which we assume to be at rest. The binding energy of the deuteron is 2.2 MeV. What energy must the incident protons have in order to induce the break-up reaction  $p + d \rightarrow p + p + n$ ?

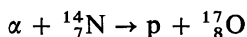
10. Consider the inelastic collision



in which  $\text{He}^+$  ions excite hydrogen atoms from the ground state to the 2p states.

- Obtain the laboratory kinetic energy of the  $\text{He}^+$  ions at the threshold of this collision.
- Calculate the recoil kinetic energy of the  $\text{H}(2p)$  particles in the laboratory system, at an angle of  $30^\circ$  and for incident  $\text{He}^+$  particles having a laboratory energy of 5 keV.

11. Consider the nuclear reaction



induced by alpha particles of 50 MeV laboratory energy. Calculate the kinetic energy in the laboratory system

- of the protons emitted in the forward direction and at a laboratory angle of  $45^\circ$ ;
- of the nuclei  ${}^{17}_8\text{O}$  recoiling at a laboratory angle of  $30^\circ$ .

[Note: The value of  $Q_{\text{if}}$  for this reaction is  $-1.18$  MeV.]

12. A beam of monochromatic photons of wavelength  $\lambda$  is scattered by a target of free electrons (Compton effect). Let  $\lambda'$  be the wavelength of a photon scattered at a laboratory angle  $\theta_L$ . Show that the wavelength shift  $\Delta\lambda = \lambda - \lambda'$  is given by  $\Delta\lambda = 2\lambda_C \sin^2 \frac{1}{2}\theta_L$ , where  $\lambda_C = h/mc$  is the Compton wavelength and  $m$  the rest mass of the electron. Obtain the laboratory recoil kinetic energy of the electron and the energy loss of the photon when  $\lambda = 1\text{\AA}(10^{-8}\text{ cm})$  and  $\theta_L = 30^\circ$ .
13. Consider a collision between two particles A and B, having masses  $m_A$  and  $m_B$ . Prove that in the laboratory system the energy  $(E_A)_L$ , the magnitude of the three-momentum  $|p_A|_L$  and that of the velocity  $|v_A|_L$  of particle A are given respectively in terms of invariant quantities by

$$(E_A)_L = \frac{1}{2m_B}(s - m_A^2 - m_B^2), \quad |p_A|_L = \frac{1}{2m_B}\sqrt{\lambda(s, m_A^2, m_B^2)}$$

and

$$|v_A|_L = \sqrt{\lambda(s, m_A^2, m_B^2)}/(s - m_A^2 - m_B^2)$$

where the quantity  $s$  is defined by eq. (2.85) and  $\lambda$  is the "triangle" function defined by eq. (2.100).

14. Consider a two-body reaction  $A + B \rightarrow C + D$  for which the Mandelstam variable  $t$  is defined by eq. (2.115).

a) Starting from eq. (2.119), find the maximum and minimum values allowed for  $t$  in terms of (fixed)  $s$  and the masses  $m_A$ ,  $m_B$ ,  $m_C$  and  $m_D$ .

b) Prove eq. (2.122).

15. Study the kinematics of pion-nucleon elastic scattering ( $s$ -channel process), together with the related  $t$ - and  $u$ -channel reactions. Determine the corresponding physical regions and represent them on the Mandelstam diagram.

16. Prove that for a two-body reaction  $A + B \rightarrow C + D$  between spinless particles the quantity  $d\sigma/dt$  is related to the center of mass differential cross section  $d\sigma/d\Omega$  by

$$\frac{d\sigma}{dt} = \frac{4\pi s}{\sqrt{\lambda(s, m_A^2, m_B^2) \lambda(s, m_C^2, m_D^2)}} \frac{d\sigma}{d\Omega}.$$

17. Consider a relativistic two-body reaction  $A + B \rightarrow C + D$ . Let  $(E_A)_L$  be the laboratory energy of particle A.

a) Show that the center of mass energies of the two outgoing particles are given respectively by

$$E_C = (E^2 + m_C^2 - m_D^2)/2E = \{E_L^2 + \gamma^2(m_C^2 - m_D^2)\}/2\gamma E_L$$

and

$$E_D = (E^2 + m_D^2 - m_C^2)/2E = \{E_L^2 + \gamma^2(m_D^2 - m_C^2)\}/2\gamma E_L$$

where  $E_L = (E_A)_L + m_B$  is the total laboratory energy,  $E = \gamma^{-1}E_L$  is the total center of mass energy and  $\gamma = (1 - V_L^2/c^2)^{-1/2}$ .

b) Let  $\theta$  be the center of mass scattering angle between the incident direction and that of the outgoing particle C. Obtain expressions for the laboratory energies  $(E_C)_L$  and  $(E_D)_L$  in terms of  $\theta$ ,  $E_C$ ,  $E_D$  and other known quantities.

18. Consider the reaction  $p + p \rightarrow d + \pi^+$ , induced by a beam of protons having a kinetic energy of 800 MeV and incident on protons at rest. The masses of the particles involved in the reaction are respectively (in MeV):  $m_p = 938.2$ ,  $m_d = 1875.4$  and  $m_{\pi^+} = 139.7$ . Let  $\theta$  be the center of mass scattering angle between the incident direction and that of the outgoing deuterons.

a) Find the center of mass kinetic energy and the magnitude of the velocity of each of the outgoing particles.

b) Obtain as a function of  $\theta$  (varying from  $0^\circ$  to  $180^\circ$  in steps of  $30^\circ$ ): the laboratory scattering angles, the kinetic energies and the ratios  $(d\sigma/d\Omega_L)/(d\sigma/d\Omega)$  for both outgoing particles.

19. Show that for a reaction (or a decay) leading to three particles  $C_1, C_2, C_3$  in the final state (with masses  $m_1, m_2, m_3$  and center of mass energies  $E_1, E_2, E_3$ ), the limiting curve of the Dalitz plot ( $E_1, E_2$ ) satisfies the equation

$$s - 2\sqrt{s}(E_1 + E_2) + 2E_1E_2 + m_1^2 + m_2^2 - m_3^2 \\ \pm 2\sqrt{(E_1^2 - m_1^2)(E_2^2 - m_2^2)} = 0.$$

20. Assume that in a certain two-body reaction  $A + B \rightarrow C + D$  one is able to detect the particles  $C$  together with their laboratory kinetic energy  $K_L$ , so that the quantity  $d\sigma/dK_L$  is known. Find the relationship between  $d\sigma/dK_L$  and the center of mass differential cross section (i) in the non-relativistic case and (ii) in the relativistic case.

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## **PART II**

### **POTENTIAL SCATTERING**

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## Potential Scattering: General Features

We begin in this chapter our study of the simplest collision problem: the non-relativistic scattering of two particles which interact through a potential  $V(\mathbf{r})$  depending only on their relative coordinate. The dynamical problem to be solved is to calculate the cross sections. This can be accomplished in two different ways. We shall first follow the *time independent* method, in which one assumes that the incident beam has been acting for a long time, so that the whole system has reached a *stationary state*. After separating the motion of the center of mass in Section 3.1, we introduce the stationary scattering wave function in Section 3.2 and show in Section 3.3 how *the cross sections are related to the asymptotic behaviour of this wave function*. An important relation, called the optical theorem is derived in Section 3.4 from the conservation of probability. Finally, we consider in Section 3.5 the scattering of wave packets. This allows us to look more closely into the physics of a scattering problem and to discuss in particular our use of stationary scattering wave functions. It also provides a useful transition towards the *time-dependent* methods which will be developed in Chapter 12 for potential scattering and in Part III for general collisions.

We assume that the reader is already familiar with the basic notions of quantum theory. However, in order to make our presentation reasonably self-contained and also to agree on terminology and notation, we have given in Appendix A a brief review of the general features of quantum mechanics.

### 3.1. Separation of the center of mass motion in a two-body problem

Let us consider a non-relativistic system of two particles A and B, with masses  $m_A$  and  $m_B$ , coordinates  $\mathbf{r}_A$  and  $\mathbf{r}_B$  measured from some fixed origin 0 (see

Fig. 3.1) and momenta  $\mathbf{P}_A, \mathbf{P}_B$ . We assume that these particles interact through a real potential  $V(\mathbf{r}_A - \mathbf{r}_B)$  which depends only upon the relative coordinate  $\mathbf{r}_A - \mathbf{r}_B$ . The classical Hamiltonian of the system is therefore given by

$$H = \mathbf{P}_A^2/2m_A + \mathbf{P}_B^2/2m_B + V(\mathbf{r}_A - \mathbf{r}_B). \quad (3.1)$$

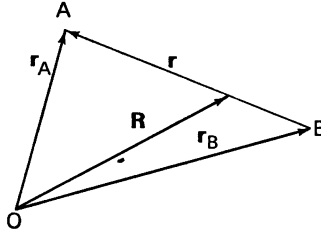


Fig. 3.1. Illustration of the vectors  $\mathbf{r}_A, \mathbf{r}_B, \mathbf{r}$  and  $\mathbf{R}$  of the text.

According to the principles of quantum mechanics, the dynamics of this two-body system is governed by the *time-dependent Schrödinger equation*

$$H\Psi(\mathbf{r}_A, \mathbf{r}_B, t) = i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_A, \mathbf{r}_B, t) \quad (3.2)$$

where  $\Psi(\mathbf{r}_A, \mathbf{r}_B, t)$  is the *wave function* of the system and the Hamiltonian operator  $H$ , written in the coordinate representation  $\{\mathbf{r}_A, \mathbf{r}_B\}$ , is obtained by making the substitutions  $\mathbf{P}_A \rightarrow -i\hbar \nabla_{\mathbf{r}_A}$  and  $\mathbf{P}_B \rightarrow -i\hbar \nabla_{\mathbf{r}_B}$  on the right-hand side of eq. (3.1). It is therefore given by [1]

$$H = -\frac{\hbar^2}{2m_A} \nabla_{\mathbf{r}_A}^2 - \frac{\hbar^2}{2m_B} \nabla_{\mathbf{r}_B}^2 + V(\mathbf{r}_A - \mathbf{r}_B) \quad (3.3)$$

and the time-dependent Schrödinger equation (3.2) may be written explicitly as

$$\left( -\frac{\hbar^2}{2m_A} \nabla_{\mathbf{r}_A}^2 - \frac{\hbar^2}{2m_B} \nabla_{\mathbf{r}_B}^2 + V(\mathbf{r}_A - \mathbf{r}_B) \right) \Psi(\mathbf{r}_A, \mathbf{r}_B, t) = i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_A, \mathbf{r}_B, t). \quad (3.4)$$

This is a partial differential equation in seven variables, namely the six spatial coordinates and the time. Fortunately, however, several important simplifications can be made. First of all, since the Hamiltonian operator (3.3) is *time-independent*, we may directly separate out the time dependence of the wave function. Indeed, we see that eq. (3.4) admits particular solutions of the form

$$\Psi(\mathbf{r}_A, \mathbf{r}_B, t) = \varphi(\mathbf{r}_A, \mathbf{r}_B) \exp\left\{-\frac{i}{\hbar} E_{\text{tot}} t\right\}, \quad (3.5)$$

namely *stationary states* for which the total energy  $E_{\text{tot}}$  of the system has a definite value. A general solution of eq. (3.4) can then be obtained as a sum of such particular solutions. Substituting the expression (3.5) of  $\Psi$  into the

Schrödinger equation (3.4), we find that the time-independent wave function  $\varphi(\mathbf{r}_A, \mathbf{r}_B)$  satisfies the equation

$$\left[ -\frac{\hbar^2}{2m_A} \nabla_{\mathbf{r}_A}^2 - \frac{\hbar^2}{2m_B} \nabla_{\mathbf{r}_B}^2 + V(\mathbf{r}_A - \mathbf{r}_B) \right] \varphi(\mathbf{r}_A, \mathbf{r}_B) = E_{\text{tot}} \varphi(\mathbf{r}_A, \mathbf{r}_B). \quad (3.6)$$

This is the *time-independent Schrödinger equation* of our two-body problem.

We now proceed to simplify eq. (3.6) by using the fact that the potential only depends on the difference of coordinates  $\mathbf{r}_A - \mathbf{r}_B$ . We introduce the relative coordinate

$$\mathbf{r} = \mathbf{r}_A - \mathbf{r}_B \quad (3.7)$$

together with the vector

$$\mathbf{R} = (m_A \mathbf{r}_A + m_B \mathbf{r}_B) / (m_A + m_B) \quad (3.8)$$

which determines the position of the center of mass of the system (see Fig. 3.1). Changing variables from the coordinates  $(\mathbf{r}_A, \mathbf{r}_B)$  to the new coordinates  $(\mathbf{r}, \mathbf{R})$ , we find that eq. (3.6) can be rewritten in terms of the new coordinates as [2]

$$\left( -\frac{\hbar^2}{2M} \nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \right) \varphi(\mathbf{R}, \mathbf{r}) = E_{\text{tot}} \varphi(\mathbf{R}, \mathbf{r}) \quad (3.9)$$

where

$$M = m_A + m_B \quad (3.10)$$

is the total mass of the system and

$$m = m_A m_B / (m_A + m_B) \quad (3.11)$$

is the reduced mass of particles A and B. In order to avoid the introduction of a new symbol we have adopted here a rather loose notation, writing  $\varphi(\mathbf{r}_A, \mathbf{r}_B) = \varphi(\mathbf{R}, \mathbf{r})$ .

We may also obtain eq. (3.9) in the following way. Let us introduce the relative momentum

$$\mathbf{p} = (m_B \mathbf{P}_A - m_A \mathbf{P}_B) / (m_A + m_B) \quad (3.12)$$

together with the total momentum

$$\mathbf{P} = \mathbf{P}_A + \mathbf{P}_B. \quad (3.13)$$

These are the conjugate momenta of the coordinates  $\mathbf{r}$  and  $\mathbf{R}$ , respectively. Since

$$\mathbf{P}_A^2 / 2m_A + \mathbf{P}_B^2 / 2m_B = \mathbf{P}^2 / 2M + \mathbf{p}^2 / 2m, \quad (3.14)$$

we can write the classical Hamiltonian (3.1) as

$$H = \mathbf{P}^2 / 2M + \mathbf{p}^2 / 2m + V(\mathbf{r}). \quad (3.15)$$

Then, making the substitutions  $\mathbf{P} \rightarrow -i\hbar \nabla_{\mathbf{R}}$  and  $\mathbf{p} \rightarrow -i\hbar \nabla_{\mathbf{r}}$ , we obtain the Hamiltonian operator in the  $\{\mathbf{R}, \mathbf{r}\}$  representation as

$$H = -\frac{\hbar^2}{2M} \nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \quad (3.16)$$

and therefore the Schrödinger equation (3.9).

Let us now analyze eq. (3.9) in more detail. Since the potential only depends on  $\mathbf{r}$ , a separation of the wave function  $\varphi(\mathbf{R}, \mathbf{r})$  can be made into a product of functions of the relative coordinates and the center of mass coordinates. In fact, eq. (3.9) has a complete set of solutions of the form [3]

$$\varphi(\mathbf{R}, \mathbf{r}) = \Phi(\mathbf{R})\psi(\mathbf{r}) \quad (3.17)$$

where the functions  $\Phi(\mathbf{R})$  and  $\psi(\mathbf{r})$  satisfy respectively the equations

$$-\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2\Phi(\mathbf{R}) = E_{\text{C.M.}}\Phi(\mathbf{R}) \quad (3.18)$$

and

$$\left(-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (3.19)$$

with

$$E_{\text{tot}} = E_{\text{C.M.}} + E. \quad (3.20)$$

We see that eq. (3.18) is a time-independent Schrödinger equation describing the center of mass as a free particle of mass  $M$  and energy  $E_{\text{C.M.}}$ . The other time-independent Schrödinger equation (3.19) corresponding to the relative motion yields a wave function  $\psi(\mathbf{r})$  which represents a particle of mass  $m$  in the potential  $V(\mathbf{r})$ . We have therefore “decoupled” the original two-body problem into two one-body problems, that of a free particle (the center of mass) and that of a single, “relative” particle of reduced mass  $m$  in a potential  $V(\mathbf{r})$ . Furthermore, if we elect to work in the C.M. system of the two colliding particles, as we shall do in what follows, we need not be concerned by the motion of the center of mass, whose coordinates are thus eliminated. The problem of the scattering of two particles interacting through a potential  $V(\mathbf{r})$  which depends only on their relative coordinate  $\mathbf{r}$  is therefore entirely equivalent, in the C.M. system, to the scattering of a particle of reduced mass  $m$  by the potential  $V(\mathbf{r})$ .

### 3.2. The stationary scattering wave function

Let us consider the non-relativistic scattering of a spinless particle of mass  $m$  by a potential  $V(\mathbf{r})$ . The time-dependent Schrödinger equation of the system, namely

$$\left(-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V(\mathbf{r})\right)\Psi(\mathbf{r}, t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) \quad (3.21)$$

admits stationary state solutions of the form

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp\left(-\frac{i}{\hbar}Et\right), \quad (3.22)$$

where the wave function  $\psi(\mathbf{r})$  is a solution of the time-independent

Schrödinger equation (3.19) and the energy  $E$  of the particle has the definite value

$$E = p^2/2m = \hbar^2 k^2/2m = mv^2/2. \quad (3.23)$$

Here

$$\mathbf{p}_i = \hbar \mathbf{k}_i = m \mathbf{v}_i \quad (3.24)$$

is the initial momentum of the particle,  $\mathbf{k}_i$  its initial wave vector and  $\mathbf{v}_i$  its initial velocity. The magnitudes of these vectors are given respectively by  $p$ ,  $k$  and  $v$ . Introducing the “reduced potential”

$$U(\mathbf{r}) = (2m/\hbar^2)V(\mathbf{r}) \quad (3.25)$$

we may rewrite eq. (3.19) as

$$[\nabla_{\mathbf{r}}^2 + k^2 - U(\mathbf{r})]\psi(\mathbf{r}) = 0. \quad (3.26)$$

We shall assume that the potential  $V(\mathbf{r})$  tends to zero faster than  $r^{-1}$  as  $r \rightarrow \infty$ , leaving the analysis of the scattering by a Coulomb potential to Chapter 6. We may then look for a particular solution of eq. (3.19) or eq. (3.26) which we shall call the stationary scattering wave function and denote by  $\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r})$ . This function satisfies the asymptotic boundary condition

$$\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} A \left( \exp(i\mathbf{k}_i \cdot \mathbf{r}) + f(\theta, \phi) \frac{\exp(ikr)}{r} \right). \quad (3.27)$$

Here  $A$  is independent of  $\mathbf{r}$  and the angles  $\theta$  and  $\phi$  are illustrated in Fig. 3.2, together with our choice of the polar  $z$ -axis along the direction of the incident wave vector  $\mathbf{k}_i$ . The origin  $O$  coincides with that of the vector  $\mathbf{r}$ .

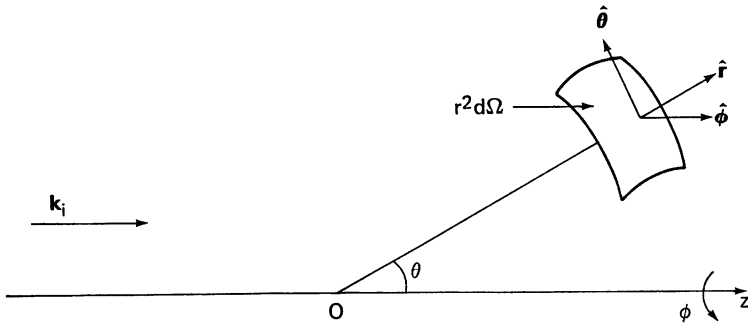


Fig. 3.2. Illustration of the coordinates used in the text.

We may easily verify that for any function  $f(\theta, \phi)$  the expression (3.27) satisfies eq. (3.19) asymptotically through terms of order  $1/r$  in the region where  $V(\mathbf{r})$  can be neglected, provided that the potential  $V(\mathbf{r})$  vanishes faster than  $r^{-1}$  as  $r \rightarrow \infty$ .

Let us now investigate the physical meaning of eq. (3.27). We see that at large distances the stationary scattering wave function  $\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r})$  is the superposition of a *plane wave* of wave vector  $\mathbf{k}_i$  and an *outgoing spherical wave*

with an amplitude depending on  $\theta$  and  $\phi$  and inversely proportional to  $r$ . That the spherical wave is an outgoing one can easily be checked by returning to the time-dependent wave function (3.22) and noting that the expression

$$\frac{1}{r} \exp\{i(kr - \omega t)\}$$

indeed describes a spherical wave with *positive phase velocity* [4]

$$dr/dt = \omega/k. \quad (3.28)$$

The physical interpretation of the quantity  $A$  and the angular function  $f$  appearing in eq. (3.27) will be discussed in the next section. We shall however postpone until Chapter 5 the proof of the existence and uniqueness of a stationary scattering wave function  $\psi_{k_i}^{(+)}$  satisfying the boundary condition (3.27). In fact, the form of the boundary condition (3.27) itself may be questioned, since the incident beam is not really a plane wave, but a narrow beam. Nevertheless, we shall show in Section 3.5, using a wave packet description, that the boundary condition (3.27) is essentially correct.

### 3.3. Cross sections

According to the definition given in Section 1.3, the quantity

$$\sigma(\Omega) d\Omega = \frac{d\sigma}{d\Omega} d\Omega \quad (3.29)$$

is the number of particles emitted per unit time and unit incident flux within the solid angle  $d\Omega$  about the direction  $\Omega(\theta, \phi)$  (see Fig. 3.2). It is therefore equal to the outgoing flux of particles scattered through the spherical surface  $r^2 d\Omega$  (for  $r \rightarrow \infty$ ), divided by the incident flux.

In order to obtain these quantities, let us consider the probability current density associated with the Schrödinger equation (3.19), namely

$$\begin{aligned} j(r) &= \frac{\hbar}{2mi} \{ \psi^*(r)(\nabla_r \psi(r)) - (\nabla_r \psi^*(r))\psi(r) \} \\ &= \text{Re} \left\{ \frac{\hbar}{mi} \psi^*(r) \nabla_r \psi(r) \right\}. \end{aligned} \quad (3.30)$$

It satisfies the continuity equation

$$\nabla_r \cdot \mathbf{j} + \partial \rho / \partial t = 0 \quad (3.31)$$

where  $\rho = |\psi|^2$  is the *probability density*. Since  $\partial \rho / \partial t = 0$  in our stationary case, eq. (3.31) reduces to

$$\nabla_r \cdot \mathbf{j} = 0. \quad (3.32)$$

Because the gradient operator  $\nabla_r$  in spherical polar coordinates is given by

$$\nabla_r = \frac{\partial}{\partial r} \hat{\mathbf{r}} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\boldsymbol{\theta}} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{\boldsymbol{\phi}} \quad (3.33)$$

where the unit vectors  $\hat{r}$ ,  $\hat{\theta}$  and  $\hat{\phi}$  are shown in Fig. 3.2, we can write the radial part of the probability current density corresponding to the wave  $\psi_{k_1}^{(+)}$  (or the radial outgoing flux through a unit surface normal to  $\hat{r}$ ) as

$$\begin{aligned} \mathbf{j} \cdot \hat{r} = \operatorname{Re} \left[ A^* A \frac{\hbar}{mi} \left\{ \exp(-ikr \cos \theta) + f^*(\Omega) \frac{\exp(-ikr)}{r} \right\} \right. \\ \left. \times \frac{\partial}{\partial r} \left\{ \exp(ikr \cos \theta) + f(\Omega) \frac{\exp(ikr)}{r} \right\} \right]. \end{aligned} \quad (3.34)$$

Consider now the incoming plane wave

$$\Phi_{k_1}(\mathbf{r}) = A \exp(ik_1 \cdot \mathbf{r}). \quad (3.35)$$

Its flux through a unit area normal to the incident wave vector  $k_1$  is given by

$$\mathbf{j}_{\text{inc}} \cdot \hat{k}_1 = \operatorname{Re} \left\{ A^* A \frac{\hbar}{mi} \exp(-ikz) \frac{d}{dz} \exp(ikz) \right\} = A^* A \frac{\hbar k}{m} = A^* A v \quad (3.36)$$

where we have used the fact that  $v = \hbar k/m$ . The radial flux of the outgoing spherical wave considered alone may be written as

$$\mathbf{j}_{\text{out}} \cdot \hat{r} = \operatorname{Re} \left\{ A^* A \frac{\hbar}{mi} f^*(\Omega) \frac{\exp(-ikr)}{r} \frac{\partial}{\partial r} \left( f(\Omega) \frac{\exp(ikr)}{r} \right) \right\}$$

or

$$\mathbf{j}_{\text{out}} \cdot \hat{r} = A^* A v \frac{1}{r^2} |f(\Omega)|^2 + \dots \quad (3.37)$$

where we have neglected terms of higher order in  $1/r$ . We may therefore rewrite eq. (3.34) as

$$\mathbf{j} \cdot \hat{r} = (\mathbf{j}_{\text{inc}} + \mathbf{j}_{\text{out}} + \mathbf{j}_{\text{int}}) \cdot \hat{r} \quad (3.38)$$

where the interference term  $\mathbf{j}_{\text{int}} \cdot \hat{r}$  is given by

$$\begin{aligned} \mathbf{j}_{\text{int}} \cdot \hat{r} = \operatorname{Re} \left\{ A^* A \frac{\hbar}{mi} \left[ \exp(-ikr \cos \theta) \frac{\partial}{\partial r} \left( f(\Omega) \frac{\exp(ikr)}{r} \right) \right. \right. \\ \left. \left. + f^*(\Omega) \frac{\exp(-ikr)}{r} \frac{\partial}{\partial r} \exp(ikr \cos \theta) \right] \right\} \\ = \operatorname{Re} \left\{ A^* A \frac{\hbar}{mi} \left[ ik f(\Omega) \frac{1}{r} \exp\{ikr(1 - \cos \theta)\} \right. \right. \\ \left. \left. + ik \cos \theta f^*(\Omega) \frac{1}{r} \exp\{-ikr(1 - \cos \theta)\} \right] + \dots \right\}. \end{aligned} \quad (3.39)$$

Again the terms of higher order in  $1/r$  have been neglected.

Let us now examine more closely the angular dependence of this interference term [5]. We see that it is completely different from that of the other two terms  $\mathbf{j}_{\text{inc}}$  and  $\mathbf{j}_{\text{out}}$ . Indeed, unless  $\theta = 0$  (forward direction scattering), it

is clear that  $j_{\text{inc}}$  oscillates very rapidly as a function of  $r$  as  $r$  becomes large. Now let us take into account the fact that the incident wave vector  $k_1$  is never sharply defined but that we have instead a superposition of waves with wave vectors in an interval  $\Delta k$  around  $k_1$  (i.e. a wave packet). The oscillatory terms may then be neglected for  $\theta \neq 0$ , since

$$\int_k^{k+\Delta k} \exp\{ikr(1 - \cos \theta)\} dk = \frac{1}{ir(1 - \cos \theta)} [\exp\{ikr(1 - \cos \theta)\}]_k^{k+\Delta k} \quad (3.40)$$

and therefore

$$\lim_{r \rightarrow \infty} \int_k^{k+\Delta k} \exp\{ikr(1 - \cos \theta)\} dk = 0, \quad \theta \neq 0. \quad (3.41)$$

Thus, except for the case  $\theta = 0$  which we shall consider in more detail below, the interference term (3.39) may be dropped so that the incident and outgoing fluxes can be computed separately. The outgoing flux of particles passing through a spherical surface element  $r^2 d\Omega$  for very large  $r$  is then given by

$$A^* A v |f(\Omega)|^2 d\Omega. \quad (3.42)$$

Dividing by the incident flux (3.36) and by  $d\Omega$  we therefore obtain the *differential cross section*

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2 \quad (3.43)$$

while the *total cross section* is given by

$$\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega}(\Omega) d\Omega. \quad (3.44)$$

The quantity  $f(\Omega)$  is called the *scattering amplitude*. Eq. (3.43) is the desired relation between the asymptotic behaviour of the wave function  $\psi_{k_1}^{(+)}$  and the differential cross section. It is of fundamental importance since it links our theoretical knowledge – contained in  $\psi_{k_1}^{(+)}$  – to the experimental quantity  $d\sigma/d\Omega$ .

Although we have indicated explicitly the dependence of the scattering amplitude on the angles  $\theta$  and  $\phi$ , it is also in general a function of the energy  $E$  of the particle (or equally well of its wave number  $k$  or of the magnitude  $p$  of its momentum or  $v$  of its velocity). Thus we may write for example

$$\frac{d\sigma}{d\Omega}(E, \theta, \phi) = |f(E, \theta, \phi)|^2 \quad (3.45)$$

or

$$\frac{d\sigma}{d\Omega}(k, \theta, \phi) = |f(k, \theta, \phi)|^2 \quad (3.46)$$



where we have used again the same notation to avoid the introduction of new symbols. Similarly, the total cross section (3.44) may be written explicitly as

$$\sigma_{\text{tot}}(E) = \int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\phi \frac{d\sigma}{d\Omega}(E, \theta, \phi) \quad (3.47)$$

with similar expressions for  $\sigma_{\text{tot}}(k)$ ,  $\sigma_{\text{tot}}(p)$ ,  $\sigma_{\text{tot}}(v)$ , etc.

At this point it is worth emphasizing the differences between scattering problems and bound state problems [6]. In the bound state case the most important quantities are the *discrete energy eigenvalues*  $E_n$ , which are obtained by solving the eigenvalue Schrödinger equation (3.19) with the appropriate boundary conditions. These include the requirement that the eigenfunctions  $\psi_n(\mathbf{r})$  corresponding to the eigenvalues  $E_n$  be square integrable, so that the normalization condition

$$\int |\psi_n(\mathbf{r})|^2 d\mathbf{r} = 1 \quad (3.48)$$

leads to the consideration of absolute probability densities  $|\psi_n|^2$ .

On the other hand, in scattering problems, the energy  $E$  is a *given* value lying in the continuous spectrum of the Hamiltonian operator  $H$ , and the basic theoretical quantity is the *scattering amplitude* which, from eq. (3.27) is related to the behaviour of the stationary wave function  $\psi_{\mathbf{k}_i}^{(+)}$  at large distances from the origin. We also note from eq. (3.27) that the wave function  $\psi_{\mathbf{k}_i}^{(+)}$  is not square integrable. A way to avoid this difficulty is to work with wave packets, as we shall illustrate in Section 3.5. Alternatively, we can adopt other types of “normalization” for our scattering wave functions, for example the delta function normalization [7] and define only *relative* probability densities. It is worth noting in connection with this point that *the cross sections are independent of the “normalization” coefficient  $A$  of eq. (3.27)*. We may therefore choose this quantity as we please. For example, if  $A = 1$  the incident plane wave has unit density in  $\mathbf{r}$  space, while the choice  $A = v^{-1/2}$  corresponds to a wave function “normalized” to unit incident flux.

### 3.4. The optical theorem

We now return to our analysis of the radial flux, but concentrate on the forward direction  $\theta = 0$ . We consider an area  $r^2 \delta\Omega$  centered about the  $z$  axis, with a small opening angle  $\delta\theta$  (see Fig. 3.3).

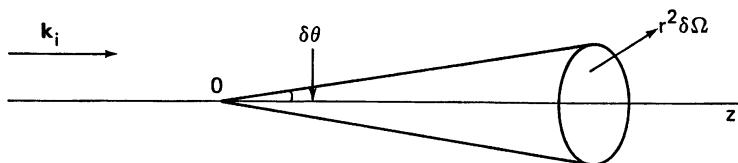


Fig. 3.3. The angle  $\delta\theta$  and area  $r^2 \delta\Omega$  of the text.

Let us integrate the expression (3.39) for the interference current over this angular interval, with all smoothly varying factors put equal to their value at  $\theta = 0$ . Since

$$\begin{aligned} & \int_{\cos \delta\theta}^1 d(\cos \theta) \exp\{ikr(1 - \cos \theta)\} \\ &= \exp(ikr) \frac{1}{-ikr} \{\exp(-ikr) - \exp(-ikr \cos \delta\theta)\} \\ &= i/kr + \text{oscillating terms,} \end{aligned} \quad (3.49)$$

we have

$$r^2 \int_{\delta\Omega} d\Omega \mathbf{j}_{\text{int}} \cdot \hat{\mathbf{r}} = -4\pi A^* A \frac{\hbar}{m} \text{Im } f(\theta = 0) \quad (3.50)$$

where we have used the fact that the scattering amplitude is independent of  $\phi$  in the forward direction.

Let us now return to the continuity equation (3.32), namely

$$\nabla_{\mathbf{r}} \cdot \mathbf{j} = 0. \quad (3.51)$$

By integrating over a sphere around the origin we deduce that

$$r^2 \int d\Omega \mathbf{j} \cdot \hat{\mathbf{r}} = 0 \quad (3.52)$$

a relation which expresses the conservation of flux, in the absence of sources or absorbers of particles within the sphere. Remembering that

$$\mathbf{j} = \mathbf{j}_{\text{inc}} + \mathbf{j}_{\text{out}} + \mathbf{j}_{\text{int}} \quad (3.53)$$

and letting  $r \rightarrow \infty$ , we obtain from eqs. (3.37), (3.38), (3.50) and (3.52)

$$A^* A \frac{\hbar}{m} \{k \int |f(\Omega)|^2 d\Omega - 4\pi \text{Im } f(\theta = 0)\} = 0 \quad (3.54)$$

where we have also used the fact that  $\int d\Omega \mathbf{j}_{\text{inc}} \cdot \hat{\mathbf{r}} = 0$ . With the help of eqs. (3.43) and (3.44), we may then write

$$\sigma_{\text{tot}} = (4\pi/k) \text{Im } f(\theta = 0). \quad (3.55)$$

This is the *optical theorem* [8], sometimes called the Bohr–Peierls–Placzek relation. It is clearly a direct consequence of the *conservation of the probability flux*. We shall see later that a relation of the type (3.55) is valid in much more general circumstances than for potential scattering. At present we simply note that eq. (3.55) arises because of the destructive *interference* between the incident and the scattered waves behind the scattering region ( $\theta \simeq 0$ ). In other words, the “shadow” cast by the target in the forward direction reduces the intensity of the incident beam, so that the scattered particles are removed from it in an amount proportional to  $\sigma_{\text{tot}}$ .

### 3.5. Potential scattering of wave packets

In this section we want to justify our use of stationary scattering wave functions and investigate in detail the boundary condition (3.27). We shall do this by considering the scattering of wave packets [9]. Although our discussion deals with the simple case of non-relativistic scattering of a spinless particle by a potential, the main results obtained can easily be generalized.

It is obvious that the use of a stationary scattering wave function

$$\psi_{k_1}^{(+)}(\mathbf{r}) \exp(-iEt/\hbar) \quad (3.56)$$

to describe the actual physical situation is an idealization. In fact, because of the inevitable spread in the direction and magnitude of the incident wave vector  $k_1$ , each particle which participates in the scattering should be represented by a wave packet built by superposing stationary waves with wave vectors  $k$  slightly different from  $k_1$ .

Let us first discuss the *free particle wave packet*, which we construct as a superposition of stationary-state eigenfunctions for the free particle. Thus we write

$$\Phi(\mathbf{r}, t) = (2\pi)^{-3/2} \int A(\mathbf{k}) \exp\{i(\mathbf{k} \cdot \mathbf{r} - \omega t)\} d\mathbf{k} \quad (3.57)$$

where [10]

$$\omega(k) = E(k)/\hbar = \hbar k^2/2m \quad (3.58)$$

and the amplitude  $A(\mathbf{k})$  can be determined by Fourier inversion if the wave packet is known at some particular time, say  $t = 0$ . Indeed

$$A(\mathbf{k}) = (2\pi)^{-3/2} \int \exp(-i\mathbf{k} \cdot \mathbf{r}) \Phi(\mathbf{r}, 0) d\mathbf{r} \quad (3.59)$$

so that  $A(\mathbf{k})$  is in fact the wave function in momentum space (or rather in "wave vector space") representing our wave packet at  $t = 0$ . We note that each individual plane wave  $\exp(i\mathbf{k} \cdot \mathbf{r} - \omega t)$  contributing to the wave packet (3.57) travels in the direction of its wave vector  $\mathbf{k}$  with constant phase velocity – the velocity of propagation of planes of equal phase –

$$v_\phi = \omega(k)/k = \hbar k/2m \quad (3.60)$$

and has a reduced wavelength  $\lambda = k^{-1}$ .

We shall normalize our wave packet in such a way that

$$\int |\Phi(\mathbf{r}, t)|^2 d\mathbf{r} = \int |A(\mathbf{k})|^2 d\mathbf{k} = 1. \quad (3.61)$$

We also assume that the experimental situation is such that the spreading (in direction and magnitude) of the wave vector  $\mathbf{k}$  is small. In that case  $A(\mathbf{k})$  exhibits a strong peak about  $\mathbf{k} = \mathbf{k}_1$ , with a small spread in wave number

$$\Delta k \ll k_1 \quad (3.62)$$

and the wave packet  $\Phi(\mathbf{r}, t)$  is practically concentrated in a region

$$\Delta r \simeq 1/\Delta k. \quad (3.63)$$

Writing

$$A(\mathbf{k}) = |A(\mathbf{k})| \exp\{i\alpha(\mathbf{k})\} \quad (3.64)$$

we have, from eq. (3.57)

$$\Phi(\mathbf{r}, t) = (2\pi)^{-3/2} \int |A(\mathbf{k})| \exp\{i[\mathbf{k} \cdot \mathbf{r} - \omega(\mathbf{k})t + \alpha(\mathbf{k})]\} d\mathbf{k}. \quad (3.65)$$

Let

$$\beta(\mathbf{k}) = \mathbf{k} \cdot \mathbf{r} - \omega(\mathbf{k})t + \alpha(\mathbf{k}) \quad (3.66)$$

be the phase of the exponential. Since  $\Phi(\mathbf{r}, t)$  clearly reaches its largest (absolute) values when the phase  $\beta$  is practically constant, we define the center of the wave packet by the condition

$$(\nabla_{\mathbf{k}}\beta(\mathbf{k}))_{\mathbf{k}=\mathbf{k}_1} = 0. \quad (3.67)$$

This point travels therefore with a uniform motion according to the law

$$\mathbf{r} = \mathbf{v}_1 t + \mathbf{r}_0 \quad (3.68)$$

where

$$\mathbf{v}_1 = (\nabla_{\mathbf{k}}\omega)_{\mathbf{k}=\mathbf{k}_1} = \hbar \mathbf{k}_1 / m \quad (3.69)$$

is the *group velocity* of the packet and

$$\mathbf{r}_0 = (-\nabla_{\mathbf{k}}\alpha(\mathbf{k}))_{\mathbf{k}=\mathbf{k}_1}. \quad (3.70)$$

More generally, if we shift the time origin at  $t = t_0$ , we have

$$\mathbf{r} = \mathbf{v}_1(t - t_0) + \mathbf{r}_0. \quad (3.71)$$

Let us examine in more detail the motion of the wave packet (3.65). We first note that, as it leaves the collimator, the packet will have a transversal width  $d$  of the order of the size of the collimator (say about  $10^{-1}$  cm). Calling  $D$  the size of the region in which the experiment is performed (see Fig. 3.4), we assume that

$$d \ll D \quad (3.72)$$

so that the scattered particles can be distinguished from the transmitted ones.

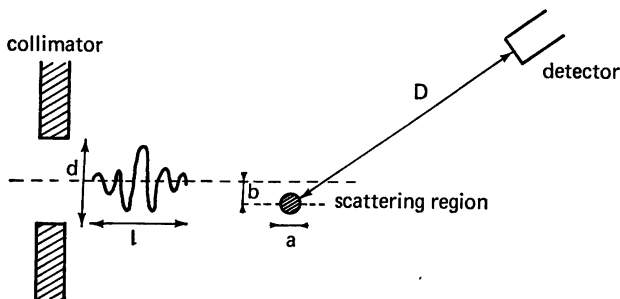


Fig. 3.4. Schematic drawing of the characteristic lengths describing the scattering of a wave packet by a potential.

Of course the wave packet also has a longitudinal width  $l$  which is directly related to the spread in energy since

$$l \simeq 1/\Delta k. \quad (3.73)$$

In what follows we shall assume that

$$d \simeq l = \Delta r. \quad (3.74)$$

We now return to the expression (3.65). Expanding  $\omega(k)$  in powers of  $(\mathbf{k} - \mathbf{k}_i)$  and keeping only the first two terms, we find with the help of eq. (3.69) that

$$\omega(k) = \omega(k_i) + \mathbf{v}_i \cdot (\mathbf{k} - \mathbf{k}_i) + \dots \quad (3.75)$$

or, since  $\mathbf{v}_i \cdot \mathbf{k}_i = 2\omega(k_i)$

$$\omega(k) = -\omega(k_i) + \mathbf{v}_i \cdot \mathbf{k} + \dots \quad (3.76)$$

Similarly, we have

$$\alpha(k) = \alpha(k_i) - \mathbf{r}_0 \cdot (\mathbf{k} - \mathbf{k}_i) + \dots \quad (3.77)$$

where we have used eq. (3.70). Thus, dropping an irrelevant constant phase vector, we may write

$$\Phi(\mathbf{r}, t) = (2\pi)^{-3/2} \exp\{i\omega(k_i)t\} \int |A(\mathbf{k})| \exp\{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{v}_i t - \mathbf{r}_0)\} d\mathbf{k} \quad (3.78)$$

so that

$$\Phi(\mathbf{r}, t) = \exp\left\{\frac{i}{\hbar}E(k_i)(t - t_0)\right\} \Phi(\mathbf{r} - \mathbf{v}_i(t - t_0), t_0). \quad (3.79)$$

Hence a free wave packet centered around the point  $\mathbf{r}_0$  at time  $t_0$  will have the *same shape* at time  $t$  and be centered about the point  $\mathbf{r} = \mathbf{v}_i(t - t_0) + \mathbf{r}_0$  (as we expect from eq. (3.71)). This result is only valid if we may neglect higher order terms in the expansions (3.75) and (3.77). In particular, we must require that

$$\frac{\hbar}{2m}(\mathbf{k} - \mathbf{k}_i)^2 t \ll 1. \quad (3.80)$$

Since

$$(\mathbf{k} - \mathbf{k}_i)^2 < (\Delta k)^2 \quad (3.81)$$

and

$$t \leq 2D/v_i = 2Dm/\hbar k_i \quad (3.82)$$

we can rewrite the condition (3.80) as

$$\{(\Delta k)^2/k_i\} D \ll 1. \quad (3.83)$$

Now, using the uncertainty relation  $\Delta r \Delta k \simeq 1$  [see eq. (3.63)] and the fact that  $\lambda_i = k_i^{-1}$ , we also have

$$(\lambda_i D)^{1/2} \ll \Delta r. \quad (3.84)$$

This requirement is easily met in most experiments dealing with microscopic systems. For example, with  $\lambda_i = 10^{-8}$  cm and  $D = 10^2$  cm, we have

$$(\lambda_i D)^{1/2} = 10^{-3} \text{ cm} \ll \Delta r \simeq 10^{-1} \text{ cm}. \quad (3.85)$$

So far, we have considered a free wave packet “centered” about the point  $\mathbf{r}_0$  at the time  $t_0$ , and whose “center” moves according to the relation (3.71). In what follows it will prove convenient to choose the time origin in such a way that at  $t = 0$  the center of the packet strikes at the position  $\mathbf{b}$  a plane perpendicular to  $\mathbf{k}_1$  and passing through the origin. The vector  $\mathbf{b}$  is called the *impact*

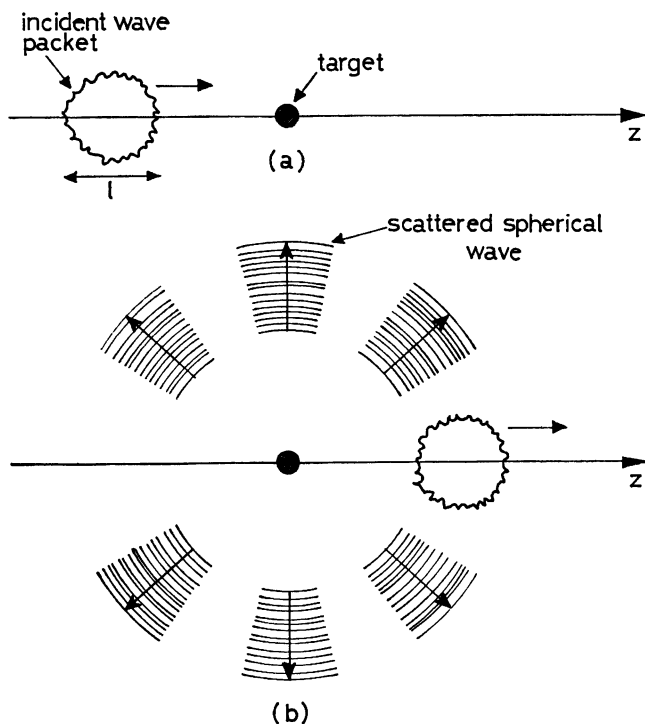


Fig. 3.5. The scattering of a wave packet by a potential (a) before the collision; (b) after the collision.

*parameter vector*; its length  $b$  is shown in Fig. 3.4. The corresponding wave packet, which we call  $\Phi_b(\mathbf{r}, t)$ , is then given from eq. (3.65) by

$$\Phi_b(\mathbf{r}, t) = (2\pi)^{-3/2} \int |A(\mathbf{k})| \exp\{i[\mathbf{k} \cdot (\mathbf{r} - \mathbf{b}) - \omega(\mathbf{k})t]\} d\mathbf{k} \quad (3.86)$$

or

$$\Phi_b(\mathbf{r}, t) = \exp\{i[\mathbf{k}_1 \cdot (\mathbf{r} - \mathbf{b}) - \omega(\mathbf{k}_1)t]\} \chi(\mathbf{r} - \mathbf{b} - \mathbf{v}_1 t) \quad (3.87)$$

where the function

$$\chi(\mathbf{r} - \mathbf{b} - \mathbf{v}_1 t) = (2\pi)^{-3/2} \int |A(\mathbf{k})| \exp\{i(\mathbf{k} - \mathbf{k}_1) \cdot (\mathbf{r} - \mathbf{b} - \mathbf{v}_1 t)\} d\mathbf{k} \quad (3.88)$$

determines the shape of the wave packet. According to eq. (3.61) we have

$$\int |\chi(\mathbf{s})|^2 d\mathbf{s} = 1. \quad (3.89)$$

It is apparent that the "center" of the wave packet  $\Phi_b(\mathbf{r}, t)$  now moves according to the law  $\mathbf{r} = \mathbf{v}_1 t + \mathbf{b}$ .

Having discussed the free particle wave packet, we now turn to a wave packet description of the scattering experiment (see Fig. 3.5). Let us denote by  $a$  the linear dimension of the scatterer. Since  $\Delta r \gg a$  in microphysics, the detailed shape of the wave packet does not affect the results of the experiment, and we may assume that all particles are described by packets of the same shape, each characterized by the quantity  $b$  which determines the motion of its center.

As in the free particle case, we now write the wave packet of the complete problem as

$$\Psi_b(\mathbf{r}, t) = (2\pi)^{-3/2} \int |A(\mathbf{k})| \exp(-i\mathbf{k} \cdot \mathbf{b}) \psi_{\mathbf{k}_1}^{(+)}(\mathbf{r}) \exp\{-i\omega(\mathbf{k})t\} d\mathbf{k} \quad (3.90)$$

where we have simply replaced the plane wave  $\exp(i\mathbf{k} \cdot \mathbf{r})$  by the stationary scattering wave  $\psi_{\mathbf{k}_1}^{(+)}(\mathbf{r})$  in eq. (3.86). Clearly  $\Psi_b(\mathbf{r}, t)$  is a solution of the time-dependent Schrödinger equation (3.21) since it is a superposition of solutions of that equation.

First of all, let us show that  $\Psi_b(\mathbf{r}, t)$  is identical to  $\Phi_b(\mathbf{r}, t)$  before the collision occurs (i.e. when  $t \rightarrow -\infty$ ). Since  $\Delta r \ll D$  and the potential tends to zero sufficiently fast as  $r \rightarrow \infty$ , the packet does not overlap the target when their centers are far apart. Therefore, we may use the asymptotic form (3.27) of the scattering wave  $\psi_{\mathbf{k}_1}^{(+)}(\mathbf{r})$  in this case and write

$$\Psi_b(\mathbf{r}, t) \rightarrow \Phi_b(\mathbf{r}, t) + \Psi_b^{\text{sc}}(\mathbf{r}, t) \quad (3.91)$$

where  $\Phi_b(\mathbf{r}, t)$  is the incident wave packet and

$$\Psi_b^{\text{sc}}(\mathbf{r}, t) = (2\pi)^{-3/2} \int |A(\mathbf{k})| \exp(-i\mathbf{k} \cdot \mathbf{b}) f(\mathbf{k}, \Omega) \frac{\exp\{i(kr - \omega(\mathbf{k})t)\}}{r} d\mathbf{k}. \quad (3.92)$$

When  $t \rightarrow -\infty$ , the phase of the integrand in eq. (3.92) cannot be stationary in the region  $\mathbf{k} \simeq \mathbf{k}_1$  where  $|A(\mathbf{k})|$  exhibits its peak. The integral (3.92) is therefore negligible and we may write

$$\Psi_b(\mathbf{r}, t) \xrightarrow{t \rightarrow -\infty} \Phi_b(\mathbf{r}, t). \quad (3.93)$$

For  $t \rightarrow +\infty$ , in the detection region, we may again write eqs. (3.91) and (3.92). In this case, however, the phase of the integrand in eq. (3.92) may be stationary in the region  $\mathbf{k} \simeq \mathbf{k}_1$  and we must examine the expression of  $\Psi_b^{\text{sc}}$  in more detail. To this end, let us write the quantity  $f(\mathbf{k}, \Omega)$  as

$$f(\mathbf{k}, \Omega) = |f(\mathbf{k}, \Omega)| \exp\{iA(\mathbf{k}, \Omega)\}. \quad (3.94)$$

Moreover, we shall assume that the function  $f(\mathbf{k}, \Omega)$  is slowly varying in a region of linear dimension  $\Delta k$  about the point  $\mathbf{k} = \mathbf{k}_1$ . Specifically, we shall write

$$|f(\mathbf{k}, \Omega)| \simeq |f(\mathbf{k}_1, \Omega)| \quad (3.95)$$

and

$$A(\mathbf{k}, \Omega) \simeq A(\mathbf{k}_i, \Omega) + \rho(\Omega) \cdot (\mathbf{k} - \mathbf{k}_i) \quad (3.96)$$

where

$$\rho(\Omega) = [\nabla_{\mathbf{k}} A(\mathbf{k}, \Omega)]_{\mathbf{k}=\mathbf{k}_i} \quad (3.97)$$

and we assume that

$$|\rho| \ll \Delta r. \quad (3.98)$$

Then if we also develop

$$\mathbf{k} = \mathbf{k}_i + \hat{\mathbf{k}}_i \cdot (\mathbf{k} - \mathbf{k}_i) + \dots \quad (3.99)$$

and use eq. (3.75), we find that

$$\Psi_b^{\text{sc}}(\mathbf{r}, t) \simeq f(\mathbf{k}_i, \Omega) \frac{\exp\{i[k_i r - \omega(k_i)t]\}}{r} \chi[\hat{\mathbf{k}}_i(r - v_i t) + \rho - \mathbf{b}]. \quad (3.100)$$

It is apparent from eq. (3.100) that if  $b > \Delta r$  the scattered wave  $\Psi_b^{\text{sc}}$  can be neglected, since the function  $\chi$  is very small. On the other hand, if  $b < \Delta r$ , then  $\Psi_b^{\text{sc}}$  represents a wave packet of outgoing spherical waves moving away from the target with the velocity  $v_i$ . In fact, we note that such a wave packet is centered at time  $t$  at the distance

$$r \simeq v_i t - \rho \cdot \hat{\mathbf{k}}_i \quad (3.101)$$

so that the quantity  $\rho \cdot \hat{\mathbf{k}}_i / v_i$  is a measure of the time delay (or advance) occurring during the passage of the scattered wave in the interaction region. The probability that a detector, placed in the direction  $\Omega \equiv (\theta, \phi)$ , will record a scattered particle is given by the probability of finding this particle within the solid angle  $(\Omega, \Omega + d\Omega)$  at a time  $t = \tau \gg \Delta r / v_i$  such that the collision process has ended. Thus we have

$$P_b(\Omega) = \int_0^\infty |\Psi_b^{\text{sc}}(\mathbf{r}, \tau)|^2 r^2 dr \quad (3.102)$$

or using eq. (3.100)

$$P_b(\Omega) = |f(\mathbf{k}_i, \Omega)|^2 \int_0^\infty |\chi[\hat{\mathbf{k}}_i(r - v_i \tau) + \rho - \mathbf{b}]|^2 dr. \quad (3.103)$$

Changing variables to  $z = r - v_i \tau$ , and using the fact that  $v_i \tau \gg \Delta r$  so that we may integrate on the  $z$  variable from  $-\infty$  to  $+\infty$ , we have

$$P_b(\Omega) = |f(\mathbf{k}_i, \Omega)|^2 \int_{-\infty}^{+\infty} |\chi(\hat{\mathbf{k}}_i z + \rho - \mathbf{b})|^2 dz. \quad (3.104)$$

We have thus far considered a particular wave packet corresponding to the impact parameter vector  $\mathbf{b}$ . For a beam of particles of unit flux, the probability of scattering in the direction  $\Omega$  is obtained by integrating the expression (3.104) over all the impact parameters  $\mathbf{b}$ . The differential cross section is therefore given by

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}_i, \Omega)|^2 \int_{-\infty}^{+\infty} dz \int d^2 \mathbf{b} |\chi(\hat{\mathbf{k}}_i z + \rho - \mathbf{b})|^2. \quad (3.105)$$



Hence, if we set

$$s = \hat{k}_i z + \rho - b \quad (3.106)$$

and use eq. (3.89), we finally obtain

$$\frac{d\sigma}{d\Omega} = |f(k_i, \Omega)|^2 \quad (3.107)$$

which is the fundamental relation (3.43).

## References and notes

- [1] We recall that the vector operator  $\nabla_{\mathbf{r}}$  is the gradient operator. In cartesian coordinates such that  $\mathbf{r} \equiv (x, y, z)$  we have  $\nabla_{\mathbf{r}} \equiv (\partial/\partial x, \partial/\partial y, \partial/\partial z)$ . The Laplacian operator  $\nabla_{\mathbf{r}}^2$  is such that  $\nabla_{\mathbf{r}}^2 = \nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{r}} = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ .
- [2] To prove that eq. (3.9) follows from eq. (3.6) we need only to look at the kinetic energy terms. Using cartesian coordinates such that  $\mathbf{r}_A \equiv (x_A, y_A, z_A)$ ,  $\mathbf{r}_B \equiv (x_B, y_B, z_B)$ ,  $\mathbf{r} \equiv (x, y, z)$  and  $\mathbf{R} \equiv (X, Y, Z)$ , we have from eqs. (3.7) and (3.8)  $x = x_A - x_B$  and  $X = (m_A x_A + m_B x_B)/(m_A + m_B)$ . Thus  $\partial/\partial x_A = \{m_A/(m_A + m_B)\}\partial/\partial X + \partial/\partial x$ ,  $\partial/\partial x_B = \{m_B/(m_A + m_B)\}\partial/\partial X - \partial/\partial x$  and therefore  $\partial^2/\partial x_A^2 = \{m_A^2/(m_A + m_B)^2\} \times \partial^2/\partial X^2 + \{2m_A/(m_A + m_B)\}\partial^2/\partial X \partial x + \partial^2/\partial x^2$ ,  $\partial^2/\partial x_B^2 = \{m_B^2/(m_A + m_B)^2\} \partial^2/\partial X^2 - \{2m_B/(m_A + m_B)\}\partial^2/\partial X \partial x + \partial^2/\partial x^2$  with similar equations for the  $y$  and  $z$  variables. Hence  $-(\hbar^2/2m_A)\nabla_{\mathbf{r}_A}^2 - (\hbar^2/2m_B)\nabla_{\mathbf{r}_B}^2 = -(\hbar^2/2M)\nabla_{\mathbf{R}}^2 - (\hbar^2/2m)\nabla_{\mathbf{r}}^2$  with  $M = m_A + m_B$  and  $m = m_A m_B/(m_A + m_B)$ , Q.E.D.
- [3] It is worth noting that the factorization property (3.17) is time-independent; if the wave function  $\phi(\mathbf{R}, \mathbf{r})$  factors at some time  $t = t_0$ , it remains factored at all times.
- [4] We recall that the phase velocity is the propagation velocity of the surface of equal phases.
- [5] We follow here the treatment of GOTTFRIED, K. (1966), *Quantum Mechanics. Volume I: Fundamentals* (Benjamin, New York) Section 12. See also: SVENSSON, B. E. Y. (1967), in Proc. 1967 CERN School of Physics at Rättvik (CERN Report 67-24, Volume II) Chapter 3.
- [6] Nevertheless, we shall see in Chapter 11 that unifying features between bound states and scattering states may be found by exploiting the analyticity properties of scattering amplitudes.
- [7] This will be illustrated in Chapters 4 and 5.
- [8] FEENBERG, E. (1932), Phys. Rev. **40**, 40.
- [9] The scattering of wave packets is studied extensively in GOLDBERGER, M. L. and K. M. WATSON (1964), *Collision Theory* (Wiley, New York) Chapter 10. See also RODBERG, L. S. and R. M. THALER (1967), *Introduction to the Quantum Theory of Scattering* (Academic Press, New York) Chapter 2; TOBOCMAN, W. and L. L. FOLDY (1959), Am. J. Phys. **27**, 483; WICHMANN, E. H. (1965), Am. J. Phys. **33**, 20; MESSIAH, A. (1968), *Quantum Mechanics* (Wiley, New York) Vol. I, Chapter 10. The wave packet treatment presented here is due essentially to F. E. Low (unpublished lecture notes).
- [10] In this section we shall denote by  $k_i$  the magnitude of the vector  $\mathbf{k}_i$  and by  $k$  the magnitude of the vector  $\mathbf{k}$  appearing in eq. (3.57). The magnitude of the velocity  $\mathbf{v}_i$  will be denoted by  $v_i$ , with  $v_i = \hbar k_i/m$ .

# The Method of Partial Waves

We have shown in Chapter 3 that the scattering amplitude and the cross sections are determined by the asymptotic behaviour of the stationary scattering wave function. In this chapter we shall learn how to use this property and to obtain explicitly the scattering amplitude and cross sections when the potential is *central* (i.e. depends only on the magnitude  $r$  of the vector  $\mathbf{r}$ ). In this case the solutions of the Schrödinger equation (3.19) may be separated in spherical polar coordinates, and a simple connection between the radial solutions and the asymptotic form of the stationary scattering wave function may be found. This procedure, which is called the *method of partial waves* [1], is exposed in Section 4.1. Two important results, namely the *optical theorem* and the *unitarity relation*, are derived in Section 4.2 within the framework of the partial wave analysis. The computation of the *phase shifts*, which play a key role in the method of partial waves, is the subject of Section 4.3. Various examples are studied in Section 4.4, while *resonances* are examined in Section 4.5. Finally, the method of partial waves is extended in Section 4.5 to the case of *complex potentials*, which allow for the removal of particles from the incident (elastic) channel.

## 4.1. The partial wave analysis

### 4.1.1. The radial equations

Let us consider the scattering of a spinless particle of mass  $m$  by a real, central potential  $V(r)$ . As in Fig. 3.2 we adopt a spherical coordinate system with the  $z$ -axis along the incident direction, while the origin  $O$  coincides with that of the vector  $\mathbf{r}$ . As shown in Fig. 4.1, the Cartesian or rectangular

coordinates of the vector  $\mathbf{r}$  are then related to its spherical polar coordinates by

$$\begin{aligned} x &= r \sin \theta \cos \phi, \\ y &= r \sin \theta \sin \phi, \\ z &= r \cos \theta. \end{aligned} \quad (4.1)$$

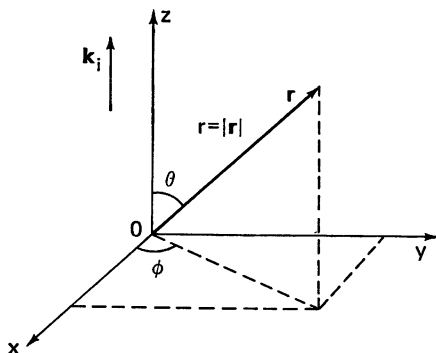


Fig. 4.1. Relation between the Cartesian and spherical polar coordinates of the vector  $\mathbf{r}$ .

The Hamiltonian operator  $H = -(\hbar^2/2m)\nabla_r^2 + V$  now reads in spherical polar coordinates

$$H = -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] + V(r) \quad (4.2)$$

and the Schrödinger time-independent equation (3.19) for the stationary scattering wave function  $\psi_{\mathbf{k}_i}^{(+)}$  can be written as

$$\begin{aligned} -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) + V(r) \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) = E \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}). \end{aligned} \quad (4.3)$$

Let us consider the *orbital angular momentum* operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad (4.4)$$

where  $\mathbf{p}$  is the momentum of the particle. We have, using the fact that  $\mathbf{p} \rightarrow -i\hbar\nabla$ , together with eqs. (4.1):

$$\begin{aligned} L_x &= y p_z - z p_y = -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) = i\hbar \left( \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right), \\ L_y &= z p_x - x p_z = -i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) = i\hbar \left( -\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right), \\ L_z &= x p_y - y p_x = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = -i\hbar \frac{\partial}{\partial \phi}. \end{aligned} \quad (4.5)$$

The operator “square of the orbital angular momentum” is then given by

$$L^2 = L_x^2 + L_y^2 + L_z^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]. \quad (4.6)$$

One easily verifies that

$$\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned} \quad (4.7)$$

and

$$[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0 \quad (4.8)$$

where

$$[A, B] = AB - BA \quad (4.9)$$

denotes the commutator of the operators  $A$  and  $B$ . From the relations (4.7) and (4.8) we deduce that one can find eigenfunctions which are common to the operators  $L^2$  and one of the components of  $L$ . These are the spherical harmonics  $Y_{lm}(\theta, \phi)$  [2] such that

$$L^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi) \quad (4.10)$$

and

$$L_z Y_{lm}(\theta, \phi) = m\hbar Y_{lm}(\theta, \phi), \quad (4.11)$$

where  $l$  and  $m$  are called respectively the *orbital angular momentum quantum number* and the *magnetic quantum number*.

We now return to the Hamiltonian (4.2) which we rewrite with the help of eq. (4.6) as

$$H = -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] + V(r) \quad (4.12)$$

so that

$$[H, L^2] = [H, L_z] = 0. \quad (4.13)$$

Because the operators  $H$ ,  $L^2$  and  $L_z$  all commute, we can look for eigenfunctions common to these three operators. We may therefore expand the scattering wave function  $\psi_{k_i}^{(+)}$  in partial waves corresponding to given values of the quantum numbers  $l$  and  $m$  as

$$\psi_{k_i}^{(+)}(k, r) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{lm}(k) R_{lm}(k, r) Y_{lm}(\theta, \phi). \quad (4.14)$$

Here we have explicitly displayed the dependence of the function  $\psi_{k_i}^{(+)}$ , of the radial functions  $R_{lm}$  and of the expansion coefficients  $c_{lm}$  on the wave number

$k = (2mE)^{1/2}/\hbar$ . The central problem of the method of partial waves is to take advantage of the expansion (4.14) in order to obtain a convenient expression of the scattering amplitude. Before we do this, however, it is necessary to analyze several important questions.

First of all, we note that by using the expansion (4.14) in the Schrödinger equation (4.3) and making use of eqs. (4.10) and (4.12) we obtain for every radial function the equation

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} \right] R_l(k, r) + V(r) R_l(k, r) = E R_l(k, r). \quad (4.15)$$

Here we have written  $R_l(k, r)$  instead of  $R_{l,m}(k, r)$  since there is no dependence on the magnetic quantum number  $m$  in eq. (4.15).

It is convenient to use the new unknown function

$$u_l(k, r) = r R_l(k, r) \quad (4.16)$$

and introduce the reduced potential  $U = 2mV/\hbar^2$  [see eq. (3.25)]. The new radial equation which we obtain from eq. (4.15) is then

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - U(r)] u_l(k, r) = 0. \quad (4.17)$$

It is worth noting that there is no loss of generality in assuming that  $u_l(k, r)$  is real, since both the real and the imaginary parts of a complex  $u_l$  would separately satisfy eq. (4.17).

#### 4.1.2. The radial equations for a free particle

In order to solve eq. (4.17) for the radial wave functions  $u_l$  it is necessary to specify the *boundary conditions* which must be satisfied by these functions. Before we do this, however, let us first examine the solutions of eq. (4.17) for  $U(r) = 0$ , namely

$$[d^2/dr^2 + k^2 - l(l+1)/r^2] y_l(k, r) = 0 \quad (4.18)$$

so that eq. (4.18) is simply the radial equation for a free particle.

Changing variables to  $\rho = kr$  and defining the function

$$f_l(\rho) = y_l/\rho \quad (4.19)$$

we see that the analogue of eq. (4.15) without interaction potential reads

$$\left[ \frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho} + \left( 1 - \frac{l(l+1)}{\rho^2} \right) \right] f_l(\rho) = 0. \quad (4.20)$$

This equation is known as the “spherical Bessel differential equation”. Particular solutions of this equation which are often used in scattering theory are the spherical Bessel function  $j_l$ , the spherical Neumann function  $n_l$  and the spherical Hankel functions  $h_l^{(1)}$  and  $h_l^{(2)}$ . The definitions and some important properties of these functions are given in Appendix C. The general solution of eq. (4.20) is then a linear combination of two linearly

independent particular solutions. Since the pairs of functions  $(j_l, n_l)$  and  $(h_l^{(1)}, h_l^{(2)})$  are linearly independent solutions of eq. (4.20) we may write the general solution  $y_l$  of eq. (4.20) as

$$y_l(k, r) = kr[C_l^{(1)}(k)j_l(kr) + C_l^{(2)}(k)n_l(kr)] \quad (4.21)$$

or

$$y_l(k, r) = kr[D_l^{(1)}(k)h_l^{(1)}(kr) + D_l^{(2)}(k)h_l^{(2)}(kr)] \quad (4.22)$$

where the two pairs of "integration constants"  $(C_l^{(1)}, C_l^{(2)})$  and  $(D_l^{(1)}, D_l^{(2)})$  may still, of course, depend on  $k$ .

The examination of the behaviour of the spherical Bessel function  $j_l(\rho)$  as  $\rho \rightarrow 0$  shows that this function is *regular* at the origin, where it is proportional to  $\rho^l$  [see Appendix C, eq. (C.11a)]. The other functions  $n_l$ ,  $h_l^{(1)}$  and  $h_l^{(2)}$  have a pole of order  $(l + 1)$  at  $\rho = 0$  and are called *irregular solutions* of eq. (4.20). By analogy, a function  $v_l(k, r)$  which is given (up to a  $k$ -dependent multiplicative factor) by

$$v_l(k, r) \sim rj_l(kr) \quad (4.23)$$

is called a *regular* solution of eq. (4.18). We note that it vanishes at the origin, namely

$$v_l(k, 0) = 0. \quad (4.24)$$

More precisely, we have

$$v_l(k, r) \underset{r \rightarrow 0}{\sim} r^{l+1}. \quad (4.25)$$

Solutions of eq. (4.18) which fail to vanish at  $r = 0$  – for example  $rn_l(kr)$ ,  $rh_l^{(1)}(kr)$  or  $rh_l^{(2)}(kr)$  – are called *irregular* solutions of that equation.

Returning to eq. (4.20), we see that the only solution [3] of that equation which is finite everywhere is (up to a  $k$ -dependent factor) the function  $j_l(kr)$ . For every positive energy value there exist therefore eigenfunctions  $j_l(kr)Y_{lm}(\theta, \phi)$  common to the *free* Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m}\nabla_r^2 \quad (4.26)$$

and to the operators  $L^2$  and  $L_z$ . We note that each solution of this kind is labelled by the value of  $k$  (varying from 0 to  $\infty$ ) and by the two indices  $l$  and  $m$  which take on discrete values. Furthermore, it may be shown that the eigenfunctions  $j_l(kr)Y_{lm}(\theta, \phi)$  constitute a complete orthogonal set, the orthogonality of the functions  $j_l(kr)$  for different values of the continuous index  $k$  being ensured by eq. (C.19) of Appendix C.

Now, the plane wave  $\exp(i\mathbf{k}_i \cdot \mathbf{r})$  which represents a free particle of well defined momentum  $\mathbf{p}_i = \hbar\mathbf{k}_i$  is clearly a solution of the Schrödinger equation

$$H_0\psi = E\psi \quad (4.27)$$

for positive values of the energy such that  $E = \hbar^2 k^2 / 2m$  (with  $k = |\mathbf{k}_i|$ ). In fact, this plane wave  $\exp(i \mathbf{k}_i \cdot \mathbf{r})$  is an eigenfunction common to the free Hamiltonian (4.26) and the (linear) momentum operator of the particle; it is labelled by the three (continuous) components of the vector  $\mathbf{k}_i$ . Since the eigenfunctions  $j_l(kr) Y_{lm}(\theta, \phi)$  form a complete set, we may develop the plane wave  $\exp(i \mathbf{k}_i \cdot \mathbf{r})$  in a series of these functions. Choosing the  $z$ -axis along the direction of  $\mathbf{k}_i$  so that  $\exp(i \mathbf{k}_i \cdot \mathbf{r}) = \exp(ikr \cos \theta)$  is independent of the azimuthal angle  $\phi$  one readily obtains the well known formula [e.g. 4]

$$\exp(i \mathbf{k}_i \cdot \mathbf{r}) \equiv \exp(ikz) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta) \quad (4.28)$$

which is the *partial wave expansion* of the plane wave  $\exp(ikz)$ . Here the functions  $P_l(\cos \theta)$  are the Legendre polynomials

$$P_l(\cos \theta) = \left( \frac{4\pi}{2l+1} \right)^{1/2} Y_{l,0}(\theta). \quad (4.29)$$

Using the addition theorem of the spherical harmonics [see eqs. (B. 39) of Appendix B], namely [5]

$$P_l(\cos \theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{lm}(\hat{\mathbf{r}}) \quad (4.30)$$

we note that eq. (4.28) may also be written as

$$\exp(i \mathbf{k}_i \cdot \mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{lm}(\hat{\mathbf{r}}), \quad (4.31)$$

a formula which is valid for any choice of  $z$ -axis. In what follows we shall continue to choose the  $z$ -axis along the direction of  $\mathbf{k}_i$ . Then, if we compare eqs. (4.14) and (4.28) and use eq. (4.29), we verify that for a free particle the radial functions  $R_{lm}(k, r)$  are indeed identical to the spherical Bessel functions  $j_l(kr)$  [up to a  $k$ -dependent factor]. Choosing this factor to be equal to one, we see that the coefficients  $c_{lm}$  of the partial wave expansion (4.14), which we denote in this case by  $c_{lm}^0$ , are given by

$$c_{lm}^0 = [4\pi(2l+1)]^{1/2} i^l \delta_{m,0}. \quad (4.32)$$

#### 4.1.3. The boundary conditions

Let us now return to the radial equation (4.17) and examine the *boundary conditions* which we must impose upon the radial functions  $u_l(k, r)$ . On the basis of the above discussion we would expect that outside the "range" [6]  $a$  of the potential we may use eq. (4.21) to express  $u_l(k, r)$  as

$$u_l(k, r) = kr [C_l^{(1)}(k) j_l(kr) + C_l^{(2)}(k) n_l(kr)], \quad r \gg a. \quad (4.33)$$

In order to investigate this question in more detail, let us assume that  $r$  is so large that the terms  $U(r)$  and  $l(l+1)/r^2$  may be neglected in eq. (4.17).

An "asymptotic" solution is then obviously of the form  $\exp(\pm ikr)$ . More precisely, we may write for large  $r$

$$u_l(k, r) = F_l(k, r) \exp(\pm ikr) \quad (4.34)$$

where  $F_l(k, r)$  is a slowly varying function of  $r$  to be determined. Substituting eq. (4.34) into eq. (4.17) we find that

$$F_l''/F_l \pm 2ikF_l'/F_l = W_l(r) \quad (4.35)$$

where we have set

$$W_l(r) = U(r) + l(l+1)/r^2 \quad (4.36)$$

and we have written  $F_l' = dF_l/dr$ ,  $F_l'' = d^2F_l/dr^2$ . Since the function  $F_l$  is slowly varying, we may drop the term  $F_l''/F_l$  in eq. (4.35) and write

$$\pm 2ikF_l'/F_l \simeq W_l(r) \quad (4.37)$$

so that for large  $r$

$$F_l(k, r) = \exp\left\{\pm \frac{1}{2ik} \int^r W_l(r') dr'\right\}. \quad (4.38)$$

Therefore, if

$$\lim_{r \rightarrow \infty} |U(r)| < \frac{M}{r^{1+\varepsilon}} \quad (4.39)$$

where  $M$  is some constant and  $\varepsilon$  is greater than zero, we deduce from eq. (4.38) that the function  $F_l$  is independent of  $r$  for  $r \rightarrow \infty$ . Thus, if the condition (4.39) is satisfied the general solution of eq. (4.17) for large  $r$  is given by

$$u_l(k, r) = B_l^{(1)}(k) e^{ikr} + B_l^{(2)}(k) e^{-ikr} \quad (4.40)$$

where  $B_l^{(1)}(k)$  and  $B_l^{(2)}(k)$  are independent of  $r$ . Using the fact that [see eqs. (C.12) of Appendix C]

$$j_l(x) \xrightarrow{x \rightarrow \infty} \frac{1}{x} \sin(x - \frac{1}{2}l\pi) \quad (4.41a)$$

$$n_l(x) \xrightarrow{x \rightarrow \infty} -\frac{1}{x} \cos(x - \frac{1}{2}l\pi) \quad (4.41b)$$

$$h_l^{(1)}(x) \xrightarrow{x \rightarrow \infty} -i \frac{\exp\{i(x - \frac{1}{2}l\pi)\}}{x} \quad (4.41c)$$

$$h_l^{(2)}(x) \xrightarrow{x \rightarrow \infty} i \frac{\exp\{-i(x - \frac{1}{2}l\pi)\}}{x} \quad (4.41d)$$

we may also rewrite eq. (4.40) in the form of eqs. (4.21) or (4.22). Thus we have, in accordance with eq. (4.33),

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} kr[C_l^{(1)}(k)j_l(kr) + C_l^{(2)}(k)n_l(kr)] \quad (4.42)$$

or

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} kr[D_l^{(1)}(k)h_l^{(1)}(kr) + D_l^{(2)}(k)h_l^{(2)}(kr)]. \quad (4.43)$$



We note, however, that the Coulomb field, which falls off like  $r^{-1}$  as  $r \rightarrow \infty$  does not satisfy the condition (4.39) so that eqs. (4.42)–(4.43) are not valid for the Coulomb interaction. We shall study the Coulomb potential separately in Chapter 6.

We may also use eqs. (4.41) to express the boundary condition (4.42) or (4.43) in slightly different manners. For example, from eqs. (4.41a) and (4.41b), we obtain

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} A_l(k) \sin[kr - \frac{1}{2}l\pi + \delta_l(k)] \quad (4.44)$$

with

$$A_l(k) = \{[C_l^{(1)}(k)]^2 + [C_l^{(2)}(k)]^2\}^{1/2} \quad (4.45a)$$

and

$$\tan \delta_l(k) = -C_l^{(2)}(k)/C_l^{(1)}(k). \quad (4.45b)$$

We note that eqs. (4.16), (4.42) and (4.45b) also imply that we may write

$$R_l(k, r) \xrightarrow{r \rightarrow \infty} \hat{A}_l(k)[j_l(kr) - \tan \delta_l(k)n_l(kr)] \quad (4.46)$$

where  $\hat{A}_l(k)$  is independent of  $r$ . We shall return shortly to the role of the “constants”  $A_l(k)$  and  $\hat{A}_l(k)$  in eqs. (4.44) or (4.46). For the moment, we note that the quantities  $\delta_l$ , which are called the *phase shifts*, display the influence of the interaction. Indeed, in the absence of interaction, the regular solution  $v_l(k, r)$  of the radial equation (4.18) (i.e. the analogue of eq. (4.17) for  $U(r) = 0$ ) is just given by  $v_l(k, r) \sim r j_l(kr)$  [see eq. (4.23)], so that

$$v_l(k, r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi). \quad (4.47)$$

Upon comparison of eqs. (4.44) and (4.47) we see that the interaction is clearly responsible for the presence of the phase shifts  $\delta_l$ . Notice that the phase shifts are measured in radians or degrees.

It is also convenient to express the boundary condition for  $u_l(k, r)$  as  $r \rightarrow \infty$  in the form of eq. (4.40) or (4.43), i.e. in terms of radially incoming  $[\exp(-ikr)]$  and outgoing  $[\exp(ikr)]$  waves. Upon comparison with eq. (4.44) we may write for example

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} \tilde{A}_l(k)[(-)^l e^{-ikr} + S_l(k) e^{ikr}] \quad (4.48)$$

with

$$\tilde{A}_l(k) = A_l(k) i^l \exp\{-i\delta_l(k)\}(-)^l/2i \quad (4.49)$$

while the coefficient of the outgoing wave is given by

$$S_l(k) = \exp\{2i\delta_l(k)\} \quad (4.50)$$

and is called an *S-matrix element* [7].

Let us now examine the boundary condition which must be satisfied by the radial functions  $u_l(k, r)$  at the origin  $r = 0$ . This boundary condition is

determined by the requirement that *all the possible physical states are described by a complete, orthogonal set of wave functions* [8]. A detailed examination of this question [e.g. 9] shows that two physically allowed solutions  $u_i(k, r)$  and  $u_i(k', r)$  must satisfy the condition

$$\lim_{r \rightarrow 0} \left\{ u_i(k, r) \frac{d}{dr} u_i^*(k', r) - u_i^*(k', r) \frac{d}{dr} u_i(k, r) \right\} = 0. \quad (4.51)$$

For a large class of potentials the requirement (4.51) may be simplified as follows. Let us assume that near the origin the interaction has the form [10]

$$U(r) = r^p(a_0 + a_1 r + \dots) \quad (4.52)$$

where  $p$  is an integer such that  $p \geq -1$ . We then expand the solution  $u_i$  in the vicinity of  $r = 0$  as

$$u_i = r^s(c_0 + c_1 r + \dots), \quad c_0 \neq 0. \quad (4.53)$$

Upon substitution of eqs. (4.52) and (4.53) in the radial equation (4.17) we find by looking at the coefficient of the lowest power of  $r$  (i.e.  $r^{s-2}$ ) that the quantity  $s$  must satisfy the *indicial equation* [e.g. 11]

$$s(s-1) - l(l-1) = 0 \quad (4.54)$$

so that  $s = l + 1$  or  $s = -l$ . The choice  $s = -l$  corresponds to *irregular solutions* which do not satisfy the condition (4.51). The other choice  $s = l + 1$  corresponds to *regular solutions* which are physically allowed. These solutions are therefore such that the condition (4.51) simplifies to [12]

$$u_i(k, 0) = 0 \quad (4.55)$$

with

$$u_i(k, r) \underset{r \rightarrow 0}{\sim} r^{l+1}. \quad (4.56)$$

We now consider the case for which the potential is more singular than  $r^{-1}$  at the origin. If the interaction is *repulsive* near  $r = 0$ , there is no special difficulty and we may continue to impose the simple condition (4.55) since obviously  $R_i(k, 0) = 0$  in this case. On the other hand, if the potential is *attractive* in the neighbourhood of the origin the nature of the singularity is important. For example, when  $p = -2$  and  $a_0 < 0$  in eq. (4.52) it may be shown [13] that physically acceptable solutions of eq. (4.17) exist only for  $a_0 > -\frac{1}{4}$ . The case for which  $p < -2$  with  $a_0 < 0$  has been studied by Case [8] with the help of the general condition (4.51). In what follows we shall consider only those interaction potentials which are less singular than  $r^{-2}$  at the origin.

#### 4.1.4. Scattering amplitude and cross sections

We now turn to the determination of the scattering amplitude. We recall that the asymptotic form of the scattering wave function  $\psi_{k_i}^{(+)}(k, \mathbf{r})$  is given by eq. (3.27), i.e.

$$\psi_{k_i}^{(+)}(k, \mathbf{r}) \underset{r \rightarrow \infty}{\rightarrow} A(k) \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) + f(k, \theta, \phi) \frac{\exp(ikr)}{r} \right], \quad (4.57)$$

where we have displayed explicitly the  $k$ -dependence of all the quantities. Using eqs. (4.28) and (4.41a), we may also write eq. (4.57) as

$$\psi_{k_i}^{(+)}(k, r) \xrightarrow{r \rightarrow \infty} A(k) \left[ \sum_{l=0}^{\infty} (2l+1) i^l \frac{\sin(kr - \frac{1}{2}l\pi)}{kr} P_l(\cos \theta) + f(k, \theta, \phi) \frac{e^{ikr}}{r} \right] \quad (4.58)$$

or, with the help of eq. (4.29),

$$\begin{aligned} \psi_{k_i}^{(+)}(k, r) \xrightarrow{r \rightarrow \infty} A(k) & \left[ \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} [4\pi(2l+1)]^{1/2} i^l \right. \\ & \times \frac{\exp\{i(kr - \frac{1}{2}l\pi)\} - \exp\{-i(kr - \frac{1}{2}l\pi)\}}{2ikr} Y_{lm}(\theta, \phi) \delta_{m,0} + f(k, \theta, \phi) \frac{e^{ikr}}{r} \left. \right]. \end{aligned} \quad (4.59)$$

On the other hand, we may also consider the partial wave expansion (4.14) for large  $r$ . Using the fact that  $R_{lm}(k, r) \equiv R_l(k, r) = r^{-1} u_l(k, r)$  together with eq. (4.44) we obtain the relation

$$\begin{aligned} \psi_{k_i}^{(+)}(k, r) \xrightarrow{r \rightarrow \infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{lm}(k) A_l(k) \frac{1}{2ir} [\exp\{i(kr - \frac{1}{2}l\pi + \delta_l)\} \\ - \exp\{-i(kr - \frac{1}{2}l\pi + \delta_l)\}] Y_{lm}(\theta, \phi). \end{aligned} \quad (4.60)$$

Upon comparison of the coefficients of the incoming spherical waves in eqs. (4.59) and (4.60) we have

$$c_{lm}(k) = \frac{A(k)}{k A_l(k)} [4\pi(2l+1)]^{1/2} i^l \exp(i\delta_l) \delta_{m,0}. \quad (4.61)$$

We note that eq. (4.61) implies that we may rewrite the partial wave expansion (4.14) as

$$\psi_{k_i}^{(+)}(k, r) = A(k) \sum_{l=0}^{\infty} \frac{\sqrt{4\pi(2l+1)}}{k A_l(k)} i^l \exp(i\delta_l) R_l(k, r) Y_{l,0}(\theta) \quad (4.62a)$$

or

$$\psi_{k_i}^{(+)}(k, r) = A(k) \sum_{l=0}^{\infty} \frac{(2l+1)}{k A_l(k)} i^l \exp(i\delta_l) R_l(k, r) P_l(\cos \theta). \quad (4.62b)$$

Next, by matching the coefficients of the outgoing spherical waves, and using eqs. (4.61) and (4.29) we find that the scattering amplitude is independent of  $\phi$  and given by

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [\exp\{2i\delta_l(k)\} - 1] P_l(\cos \theta). \quad (4.63)$$

We may also rewrite eq. (4.63) in the form

$$f(k, \theta) = \sum_{l=0}^{\infty} (2l+1) a_l(k) P_l(\cos \theta) \quad (4.64)$$

where the *partial wave amplitudes*  $a_l(k)$  are such that

$$a_l(k) = \frac{1}{2ik} [\exp\{2i\delta_l(k)\} - 1] = \frac{1}{2ik} [S_l(k) - 1]. \quad (4.65)$$

Thus the knowledge of the phase shifts enables one to obtain the scattering amplitude. We will return in Section 4.3 to the actual calculation of phase shifts. For the moment, we note that we may also rewrite eq. (4.63) as

$$f(k, \theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp\{i\delta_l(k)\} \sin \delta_l(k) P_l(\cos \theta) \quad (4.66)$$

while eq. (4.65) becomes

$$a_l(k) = \frac{1}{k} \exp\{i\delta_l(k)\} \sin \delta_l(k). \quad (4.67)$$

According to the fundamental relation (3.43), the differential scattering cross section is given by

$$\begin{aligned} \frac{d\sigma}{d\Omega}(k, \theta) = |f(k, \theta)|^2 &= \frac{1}{k^2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)(2l'+1) \exp\{i[\delta_l(k) - \delta_{l'}(k)]\} \\ &\times \sin \delta_l(k) \sin \delta_{l'}(k) P_l(\cos \theta) P_{l'}(\cos \theta). \end{aligned} \quad (4.68)$$

The total cross section is then obtained as

$$\sigma_{\text{tot}}(k) = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega}(k, \theta) \sin \theta d\theta. \quad (4.69)$$

Since [see eq. (B.5) of Appendix B]

$$\int_{-1}^{+1} P_l(x) P_{l'}(x) dx = \frac{2}{2l+1} \delta_{ll'}, \quad (4.70)$$

only the terms with  $l = l'$  arising from the double sum (4.68) contribute to the integral (4.69), so that

$$\sigma_{\text{tot}}(k) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(k) = \sum_{l=0}^{\infty} \sigma_l(k) \quad (4.71)$$

where each partial wave cross section  $\sigma_l(k)$  is given by

$$\sigma_l(k) = \frac{4\pi}{k^2} (2l+1) \sin^2 \delta_l(k). \quad (4.72)$$

We note that the maximum contribution of each partial wave to the total cross section is given by

$$\sigma_l^{\text{max}}(k) = \frac{4\pi}{k^2} (2l+1) \quad (4.73)$$

and occurs when

$$\delta_l(k) = (n + \frac{1}{2})\pi, \quad n = 0, \pm 1, \pm 2, \dots \quad (4.74)$$

On the contrary, when  $\delta_l(k) = n\pi$  there is no contribution to the scattering from that partial wave at the energy  $E = \hbar^2 k^2 / 2m$ .

It is apparent from the above formulae that the method of partial waves is most useful when only a small number of partial waves contribute to the scattering. This situation arises at *low incident energies*. More precisely, if  $a$  is the “range” [6] of the potential and  $k$  the wave number of the particle, only those partial waves will be important for which

$$l \lesssim ka. \quad (4.75)$$

We shall shortly obtain this condition by using a simple semi-classical argument. For the moment, we note that the first and most important maximum of the free radial wave function  $j_l(kr)$  occurs approximately at  $r_0 = l/k$ , while for small  $r$  the function  $j_l$  is small and increases as  $r^l$  (see Appendix C). Therefore, if  $a \ll l/k$ , the function  $j_l$  will be very small in the scattering region, and the corresponding phase shift  $\delta_l$  will be negligible. We may then cut off the partial wave series approximately at  $l_{\max} = ka$ . Thus, if

$$ka < 1 \quad (4.76)$$

we need only calculate a small number of phase shifts in order to obtain the scattering amplitude.

The physical explanation of this fact is very simple. Indeed, if we return to the radial equation (4.17), we see that the “effective potential” is just  $U_{\text{eff}}(r) = U(r) + l(l+1)/r^2$  and that the centrifugal barrier term  $l(l+1)/r^2$  becomes more and more important as  $l$  increases. Hence, when  $l$  grows, the incident particle needs more and more kinetic energy to overcome the repulsion of the centrifugal term in order to probe the region where the potential acts. We therefore expect that at low bombarding energies only a few low partial waves will affect the scattering significantly.

Two important reservations should be made about the above discussion. Firstly, the potential should not decrease too slowly at large distances. Indeed, if the potential falls off slowly at large  $r$  the role of the centrifugal barrier is less important and substantial scattering can be caused by the long tail of the interaction. We shall therefore require that the potential has a finite “range” [6]. Secondly, we have not taken into account the possibility of resonance phenomena which – at a given energy – may considerably enhance the scattering in a particular partial wave. We shall study resonance scattering in Section 4.5, but turn now to a semi-classical description of the collision which illustrates qualitatively the discussion following eq. (4.75).

#### 4.1.5. Semi-classical description of a collision

Let us first consider the scattering of *classical* particles having an incident momentum  $p_1$  by a central force of finite range  $a$  (see Fig. 4.2). This, of course, represents always an idealization in which the quantum features of the collision are ignored. In that case the concept of *trajectory* may be used.

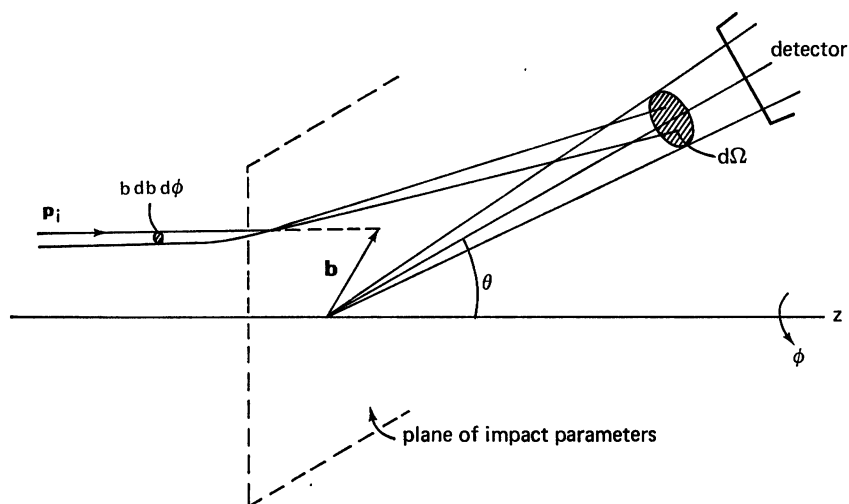


Fig. 4.2. The scattering of a classical particle.

The position of each incident particle can then be defined by the cylindrical coordinates  $(b, \phi, z)$ . The quantity  $b$  is called the *impact parameter*, while the vector  $\mathbf{b} \equiv (b, \phi)$  is the *impact parameter vector*. From the definition of Section 3.1, we note that the quantity  $d\sigma$  is equal to the area which, lying in a plane perpendicular to  $\mathbf{p}_i$ , is crossed by the particles scattered into the solid angle  $d\Omega$  centered around the direction  $\Omega(\theta, \phi)$ . Thus we have, classically

$$d\sigma_{cl} = b db d\phi = b \left| \frac{db}{d(\cos \theta)} \right| |d(\cos \theta)| d\phi \quad (4.77)$$

and since

$$d\Omega = \sin \theta d\theta d\phi = |d(\cos \theta)| d\phi \quad (4.78)$$

we may write the *classical differential cross section* as

$$\frac{d\sigma_{cl}}{d\Omega} = b \left| \frac{db}{d(\cos \theta)} \right| = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right|. \quad (4.79)$$

We remark that the quantity  $d\sigma_{cl}/d\Omega$  may be obtained as soon as  $b$  is known as a function of  $\theta$ . The determination of  $b(\theta)$  is a well known problem of classical scattering theory [e.g. 14]. We note that a classical particle will be deflected or not according to whether its impact parameter  $b$  is such that  $b < a$  or  $b > a$ . Moreover, the angular momentum  $L = bp$  (with  $p = |\mathbf{p}_i|$ ) is a constant of the motion.

Let us now go over to the quantum mechanical case. We shall require that  $ka \gg 1$ , so that the reduced de Broglie wavelength  $\lambda = k^{-1}$  of the particle

is small with respect to  $a$ . We are then in a “semi-classical” situation and we may write

$$b = L/p \simeq \sqrt{l(l+1)}/k. \quad (4.80)$$

By analogy with the classical situation, we expect substantial scattering only when

$$b \lesssim a \quad \text{or} \quad \sqrt{l(l+1)} \simeq l \lesssim ka \quad (4.81)$$

so that we recover the condition (4.75). It is important to note that the semi-classical “derivation” given here only holds when  $ka \gg 1$ . In fact, the discussion following eq. (4.75) shows that this restriction is unnecessary and that (except for resonances) the condition (4.75) is quite general.

#### 4.1.6. The scattering wave function

Let us now return to the partial wave expansion (4.62) of the scattering wave function  $\psi_{k_1}^{(+)}$ . In terms of the radial wave functions  $u_l(k, r)$ , we may write

$$\psi_{k_1}^{(+)}(k, r) = A(k) \sum_{l=0}^{\infty} \frac{\sqrt{4\pi(2l+1)}}{A_l(k)} i^l \exp(i\delta_l) \frac{u_l(k, r)}{kr} Y_{l,0}(\theta) \quad (4.82a)$$

or

$$\psi_{k_1}^{(+)}(k, r) = A(k) \sum_{l=0}^{\infty} \frac{2l+1}{A_l(k)} i^l \exp(i\delta_l) \frac{u_l(k, r)}{kr} P_l(\cos \theta) \quad (4.82b)$$

where the functions  $u_l(k, r)$  exhibit the asymptotic behaviour (4.44). Hence

$$\psi_{k_1}^{(+)}(k, r) \xrightarrow{r \rightarrow \infty} A(k) \sum_{l=0}^{\infty} (2l+1) i^l \exp(i\delta_l) \frac{\sin(kr - \frac{1}{2}l\pi + \delta_l)}{kr} P_l(\cos \theta) \quad (4.83)$$

and we see that the coefficients  $A_l(k)$  have no influence on the scattering [15]. They merely fix the “normalization” [16] of the radial functions. The following “normalizations” are often used [17]

$$\text{i) } u_l(k, r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi + \delta_l), \quad (4.84a)$$

or

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi) \cos \delta_l + \cos(kr - \frac{1}{2}l\pi) \sin \delta_l, \quad (4.84b)$$

$$\text{ii) } u_l(k, r) \xrightarrow{r \rightarrow \infty} \frac{1}{k} \sin(kr - \frac{1}{2}l\pi + \delta_l) \quad (4.85a)$$

so that

$$R_l(k, r) \xrightarrow{r \rightarrow \infty} \frac{1}{kr} \sin(kr - \frac{1}{2}l\pi + \delta_l), \quad (4.85b)$$

or

$$R_l(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) \cos \delta_l - n_l(kr) \sin \delta_l; \quad (4.85c)$$

$$\text{iii) } u_l(k, r) \xrightarrow{r \rightarrow \infty} \frac{1}{k} [\sin(kr - \frac{1}{2}l\pi) + \cos(kr - \frac{1}{2}l\pi) \tan \delta_l] \quad (4.86a)$$

so that

$$R_l(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) - \tan \delta_l n_l(kr). \quad (4.86b)$$

We also note that eq. (4.82b) may be written in the simple form

$$\psi_{k_1}^{(+)}(k, r) = r^{-1} \sum_{l=0}^{\infty} \chi_l(k, r) P_l(\cos \theta) \quad (4.87)$$

where we have introduced the new functions  $\chi_l(k, r)$  such that

$$\chi_l(k, r) = \bar{A}_l(k) u_l(k, r) \quad (4.88a)$$

with

$$\bar{A}_l(k) = \frac{A(k)}{k A_l(k)} (2l + 1) i^l \exp(i\delta_l). \quad (4.88b)$$

Therefore, upon using eq. (4.44), we have

$$\chi_l(k, r) \xrightarrow{r \rightarrow \infty} \frac{A(k)}{k} (2l + 1) i^l \exp(i\delta_l) \sin(kr - \frac{1}{2}l\pi + \delta_l). \quad (4.89)$$

Finally, for further reference, we note that the relation (4.83) may also be written in terms of incoming and outgoing spherical waves as

$$\begin{aligned} \psi_{k_1}^{(+)}(k, r) &\xrightarrow{r \rightarrow \infty} A(k) \sum_{l=0}^{\infty} (2l + 1) \frac{i}{2kr} \\ &\times [(-)^l \exp(-ikr) - \exp(2i\delta_l) \exp(ikr)] P_l(\cos \theta) \end{aligned} \quad (4.90a)$$

or, using eqs. (4.41c) and (4.41d),

$$\begin{aligned} \psi_{k_1}^{(+)}(k, r) &\xrightarrow{r \rightarrow \infty} A(k) \sum_{l=0}^{\infty} (2l + 1) \frac{1}{2} i^l \\ &\times [h_l^{(2)}(kr) + \exp(2i\delta_l) h_l^{(1)}(kr)] P_l(\cos \theta). \end{aligned} \quad (4.90b)$$

## 4.2. Optical theorem and unitarity relation

Let us return to the relation (4.66). Since  $P_l(1) = 1$  we obtain in the forward direction [18]

$$f(\theta = 0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \exp(i\delta_l) \sin \delta_l \quad (4.91)$$

so that

$$\text{Im } f(\theta = 0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l. \quad (4.92)$$

Hence, upon comparison with eq. (4.71), we find that

$$\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im } f(\theta = 0), \quad (4.93)$$

which is the *optical theorem* (3.55).



More generally, one can readily obtain the *unitarity relation* [19]

$$\text{Im } f(\theta) = \frac{k}{4\pi} \int f^*(\theta') f(\theta_0) d\Omega', \quad (4.94)$$

where  $\theta_0$  is the angle between the directions  $(\theta, 0)$  and  $(\theta', \phi')$ , as shown in Fig. 4.3. Indeed, let us write from eq. (4.66)

$$f(\theta_0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp(i\delta_l) \sin \delta_l P_l(\cos \theta_0) \quad (4.95a)$$

and

$$f^*(\theta') = \frac{1}{k} \sum_{l'=0}^{\infty} (2l'+1) \exp(-i\delta_{l'}) \sin \delta_{l'} P_{l'}(\cos \theta'). \quad (4.95b)$$

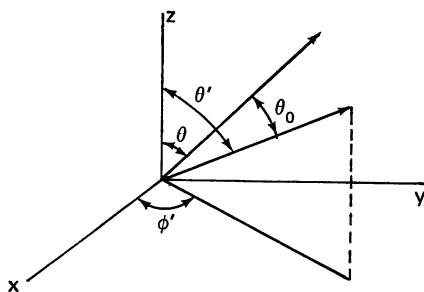


Fig. 4.3. Illustration of the angles involved in the unitarity relation (4.94).

But, according to the “addition theorem” of spherical harmonics [see eq. (4.30)], we have

$$P_l(\cos \theta_0) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi) \quad (4.96a)$$

while [see eq. (4.29)]

$$P_{l'}(\cos \theta') = \left( \frac{4\pi}{2l'+1} \right)^{1/2} Y_{l',0}(\theta'). \quad (4.96b)$$

Hence, using eqs. (4.95) and (4.96), we may write

$$\begin{aligned} \frac{k}{4\pi} \int f^*(\theta') f(\theta_0) d\Omega' &= \frac{1}{k} (4\pi)^{1/2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} \sum_{m=-l}^{+l} (2l'+1)^{1/2} \exp\{i(\delta_l - \delta_{l'})\} \\ &\quad \times \sin \delta_l \sin \delta_{l'} Y_{lm}(\theta, \phi) \int Y_{lm}^*(\theta', \phi') Y_{l',0}(\theta') d\Omega'. \end{aligned}$$

Now, because of the orthonormality property of the spherical harmonics, this equation becomes

$$\frac{k}{4\pi} \int f^*(\theta') f(\theta_0) d\Omega' = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l \left[ \left( \frac{4\pi}{2l+1} \right)^{1/2} Y_{l,0}(\theta) \right]$$

or

$$\frac{k}{4\pi} \int f^*(\theta') f(\theta_0) d\Omega' = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l P_l(\cos \theta). \quad (4.97)$$

On the other hand, we deduce from eq. (4.66) that

$$\text{Im } f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l P_l(\cos \theta). \quad (4.98)$$

Comparing eqs. (4.97) and (4.98), we then obtain eq. (4.94). It is clear that the unitarity relation (4.94) reduces to the optical theorem (4.93) when  $\theta = 0$ . Furthermore, we may use eq. (4.54) to write the unitarity relation in terms of partial wave amplitudes as

$$\text{Im } a_l(k) = k |a_l(k)|^2. \quad (4.99)$$

### 4.3. The phase shifts

We have shown in Section 4.1 that the knowledge of the phase shifts allows one to obtain the scattering amplitude by means of the important relation (4.63). In this section we shall study these phase shifts in more detail.

#### 4.3.1. Relation between the phase shifts and the potential

Let us first establish some general relationships between the phase shifts and the interaction potential. For this purpose, we consider the scattering by two reduced potentials  $U(r)$  and  $\bar{U}(r)$ , with respective radial equations [we omit here the explicit  $k$ -dependence of the radial functions]

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - U(r)]u_l(r) = 0 \quad (4.100a)$$

and

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - \bar{U}(r)]\bar{u}_l(r) = 0. \quad (4.100b)$$

We shall assume that the functions  $u_l(r)$  and  $\bar{u}_l(r)$  are “normalized” according to eq. (4.86a), namely

$$u_l(r) \xrightarrow{r \rightarrow \infty} \frac{1}{k} [\sin(kr - \frac{1}{2}l\pi) + \cos(kr - \frac{1}{2}l\pi) \tan \delta_l], \quad (4.101a)$$

$$\bar{u}_l(r) \xrightarrow{r \rightarrow \infty} \frac{1}{k} [\sin(kr - \frac{1}{2}l\pi) + \cos(kr - \frac{1}{2}l\pi) \tan \bar{\delta}_l]. \quad (4.101b)$$

The Wronskian of the two solutions  $u_l$  and  $\bar{u}_l$  is defined as

$$W(u_l, \bar{u}_l) = u_l \bar{u}_l' - u_l' \bar{u}_l \quad (4.102)$$

where the prime denotes a derivative with respect to the variable  $r$ . Multiplying eq. (4.100a) by  $\bar{u}_l$ , eq. (4.100b) by  $u_l$  and subtracting term by term, we obtain

$$\bar{u}_l u_l'' - u_l \bar{u}_l'' - (U - \bar{U}) u_l \bar{u}_l = 0$$

or

$$\frac{d}{dr} W(u_l, \bar{u}_l) = - (U - \bar{U}) u_l \bar{u}_l. \quad (4.103)$$

Upon integration over the variable  $r$  in the interval  $(a, b)$ , we deduce that

$$[W(u_l, \bar{u}_l)]_a^b = - \int_a^b \bar{u}_l(r) [U(r) - \bar{U}(r)] u_l(r) dr. \quad (4.104)$$

Choosing  $a = 0$  and  $b = \infty$  and remembering that  $u_l(0) = \bar{u}_l(0) = 0$  we find with the help of eqs. (4.101) that

$$\tan \delta_l - \tan \bar{\delta}_l = - k \int_0^\infty \bar{u}_l(r) [U(r) - \bar{U}(r)] u_l(r) dr \quad (4.105)$$

provided that  $U(r)$  and  $\bar{U}(r)$  tend to zero faster than  $r^{-1}$  when  $r \rightarrow \infty$ . We also require that the potentials  $U(r)$  and  $\bar{U}(r)$  should not be more singular than  $r^{-2}$  at the origin, since  $u_0(r) \sim r$  as  $r \rightarrow 0$  [see eq. (4.56)]. For the particular case  $\bar{U} = 0$  we deduce from eq. (4.105) the important integral representation

$$\tan \delta_l = - k \int_0^\infty j_l(kr) U(r) R_l(r) r^2 dr \quad (4.106)$$

where the radial function  $R_l(r)$  is normalized according to eq. (4.86b).

The relation (4.105) provides a way of investigating the dependence of the phase shifts on the potential. Indeed, let us suppose that the potential depends parametrically on a quantity  $\lambda$  (which may be thought of as a coupling constant or a "strength parameter") in such a way that  $U = U(\lambda, r)$  while  $\bar{U} = U(\bar{\lambda}, r)$ . Let  $d\lambda = \bar{\lambda} - \lambda$  be an arbitrary small quantity. Then, by eq. (4.105), we have

$$\frac{d}{d\lambda} \delta_l = - k \int_0^\infty [u_l(\lambda, r)]^2 \frac{\partial U(\lambda, r)}{\partial \lambda} dr \quad (4.107)$$

where we have neglected higher order terms in  $d\lambda$ . Hence, if the variation of the potential  $\partial U / \partial \lambda$  has the same sign for any value of  $r$ , the corresponding variation of the phase shift has the opposite sign.

By using eq. (4.107) we may give an *absolute* definition of phase shifts. Indeed, until now the phase shifts were only defined modulo  $\pi$ , but we can remove this ambiguity by requiring that  $\delta_l = 0$  when  $U = 0$  [20]. By varying smoothly the potential (i.e. varying the parameter  $\lambda$  in a continuous way) from  $U(\lambda_1, r) = 0$  to  $U(\lambda_2, r) = U(r)$  we may then generate progressively the phase shifts  $\delta_l$  corresponding to a potential  $U(r)$ . We note, however, that this procedure cannot be used for the particular values  $k = 0$  and  $k = \infty$ , where eq. (4.107) has no meaning. In fact, we shall prove in Section 11.3 an important theorem, due to Levinson [21] which implies that the phase shifts  $\delta_l$  at  $k = 0$  do *not* vary smoothly as a function of the strength parameter  $\lambda$ .

Adopting this above absolute definition of the phase shifts, we see from eq. (4.107) that if the potential is repulsive (i.e. positive for all  $r$ ), then  $\delta_l < 0$ .

Any increase in this potential yields a smaller (more negative) phase shift. Conversely, a purely attractive potential (negative for all  $r$ ) yields a phase shift  $\delta_l > 0$ . By making this potential more attractive, we increase  $\delta_l$ . These features may easily be understood physically. We first note from eq. (4.47) that the free solution  $v_l(k, r)$  has nodes at

$$r = \frac{1}{k}(n\pi + \frac{1}{2}l\pi) \quad (4.108)$$

while from eq. (4.44) we infer that the corresponding nodes of the radial function  $u_l(k, r)$  occur in the asymptotic region at

$$r = \frac{1}{k}(n\pi + \frac{1}{2}l\pi - \delta_l). \quad (4.109)$$

Now, for repulsive potentials we expect that the radial wave  $u_l(k, r)$  should be “pushed out” with respect to the free radial wave  $v_l(k, r)$ . Thus the zeros given by eq. (4.109) should be displaced with respect to those of eq. (4.108) by a *positive* amount ( $-\delta_l/k$ ). Hence  $\delta_l < 0$  in this case [see Fig. 4.4(a)]. By the same reasoning we see that for an attractive potential the radial wave  $u_l(k, r)$  is “pulled in” with respect to  $v_l(k, r)$  so that  $\delta_l > 0$ , as shown on Fig. 4.4(b).

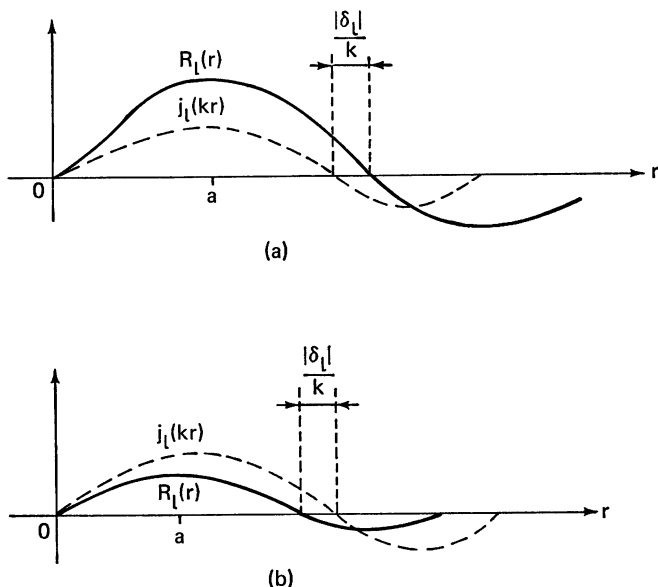


Fig. 4.4. Schematic representation of the effect on the free radial wave  $j_l(kr)$  of (a) a repulsive (positive) potential, (b) an attractive (negative) potential.

We have already seen above that if  $\delta_l(k) = n\pi$  for particular values of  $l$  and  $k$ , there will be no scattering from that partial wave at the energy  $E = \hbar^2 k^2 / 2m$  considered. For example, it may happen that an attractive potential is strong

enough to yield an  $s$ -wave ( $l = 0$ ) [22] phase shift  $\delta_0 = \pi$  at a particular low energy ( $ka \ll 1$ ) such that the other phase shifts may be neglected. In that case there will be essentially no scattering at that energy. Such a phenomenon, called the *Ramsauer–Townsend effect*, has been observed in low-energy collisions of electrons with rare-gas atoms.

#### 4.3.2. The calculation of the phase shifts

We now turn to the actual computation of the phase shifts. They are obtained by solving the radial equations (4.15) or (4.17) – numerically if necessary – subject to the boundary conditions discussed in Section 4.1.3 [23]. In particular, the solution obtained inside the range of the potential must go over smoothly to the “asymptotic” solution, valid outside the range of the interaction.

When the potential has a *strict finite range*, i.e. vanishes for  $r > a$ , one can divide the domain of the variable  $r$  into an internal region ( $r < a$ ) and an external region ( $r > a$ ). The boundary conditions at  $r = a$  are then that both  $R_l$  and  $dR_l/dr$  [or  $u_l$  and  $du_l/dr$ ] be continuous [24] at  $r = a$ . Equivalently, we may require that the logarithmic derivatives  $[R_l^{-1}(dR_l/dr)]$  or  $[u_l^{-1}(du_l/dr)]$  be continuous at  $r = a$ . Now the *exterior* solution may be written for example as [see eq. (4.46)]

$$R_l(k, r) = \hat{A}_l(k)[j_l(kr) - \tan \delta_l n_l(kr)]. \quad (4.110)$$

Thus, if we denote by

$$\gamma_l = [R_l^{-1}(dR_l/dr)]_{r=a} \quad (4.111)$$

the value of the logarithmic derivative of the interior solution  $R_l(k, r)$  at  $r = a$  [25], we find that

$$\gamma_l(k) = \frac{k[j'_l(ka) - \tan \delta_l(k) n'_l(ka)]}{j_l(ka) - \tan \delta_l(k) n_l(ka)}, \quad (4.112)$$

where we have defined  $j'_l(ka) = [dj_l(x)/dx]_{x=ka}$  and  $n'_l(ka) = [dn_l(x)/dx]_{x=ka}$ . Hence

$$\tan \delta_l(k) = \frac{kj'_l(ka) - \gamma_l(k)j_l(ka)}{kn'_l(ka) - \gamma_l(k)n_l(ka)}. \quad (4.113a)$$

This formula will be illustrated in Section 4.4 in the case of a square well potential. A similar formula may evidently be obtained in terms of the logarithmic derivative of the interior solution  $u_l(k, r)$  at  $r = a$  [26].

If the potential does not vanish identically beyond a certain value of  $r$ , but has nevertheless a “range”  $a$  [6], one chooses a distance  $d \gtrsim a$  at which the influence of the potential is negligible. The value of the logarithmic derivative of the interior solution is then matched at  $r = d$  with that of the exterior (free) solution [27] so that in this case

$$\tan \delta_l(k) = \frac{kj'_l(kd) - \gamma_l(k)j_l(kd)}{kn'_l(kd) - \gamma_l(k)n_l(kd)}. \quad (4.113b)$$

It is clear that in performing calculations of this type one must check that the phase shifts so obtained are insensitive (within the accuracy required) to any increase in the quantity  $d$ . In what follows, we shall assume for simplicity that  $d = a$ . The potentials having a strict finite range and those having a "range" will then be treated on the same footing.

#### 4.3.3. Behaviour of the phase shifts at low energies. Scattering length.

We may use the properties of the functions  $j_l$  and  $n_l$  given in Appendix C to predict the behaviour of the phase shifts at low energies. Indeed, let us define the dimensionless quantity

$$q_l(k) = \frac{kj'_l(ka)/j_l(ka)}{\gamma_l(k)}. \quad (4.114)$$

Clearly, if the interaction is negligible, we have  $R_l(kr) \sim j_l(kr)$  and  $q_l = 1$ . Now, using the properties (C. 10) of the functions  $j_l$  and  $n_l$ , we deduce from eqs. (4.113) and (4.114) that for  $ka \ll l$

$$\tan \delta_l(k) \simeq \frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \frac{q_l(k) - 1}{\{(l+1)/l\}q_l(k) + 1}, \quad l > 0. \quad (4.115)$$

Moreover, we note from eqs. (C.10) that the quantity  $\gamma_l^0(k) = kj'_l(ka)/j_l(ka)$  [i.e. the ratio of slope to value of the free radial function at  $r = a$ ] is given for  $ka \ll l$  by

$$\gamma_l^0(k) = a^{-1}[l + \mathcal{O}(k^2a^2)], \quad l > 0 \quad (4.116)$$

so that we deduce from eq. (4.114) that

$$q_l(k) = [a\gamma_l(k)]^{-1}[l + \mathcal{O}(k^2a^2)], \quad l > 0. \quad (4.117)$$

For  $l = 0$  and  $ka \ll 1$ , we have instead

$$\tan \delta_0(k) \simeq ka \frac{q_0(k) - 1}{1 - 3(ka)^{-2}q_0(k)} \quad (4.118)$$

with

$$q_0(k) = [a\gamma_0(k)]^{-1}[-\frac{1}{3}(ka)^2 + \mathcal{O}(k^4a^4)], \quad l = 0. \quad (4.119)$$

Hence, for both cases  $l = 0$  and  $l > 0$ , we may write [28]

$$\tan \delta_l \simeq \frac{(ka)^{2l+1}}{D_l} \frac{l - a\gamma_l(k)}{l + 1 + a\gamma_l(k)} \quad (4.120)$$

and

$$\tan \delta_l \xrightarrow{k \rightarrow 0} \frac{(ka)^{2l+1}}{D_l} \frac{l - a\hat{\gamma}_l}{l + 1 + a\hat{\gamma}_l} \quad (4.121)$$

where we have defined

$$\begin{aligned} D_l &= (2l+1)!!(2l-1)!!, \quad l > 0 \\ D_0 &= 1 \end{aligned} \quad (4.122)$$

and

$$\hat{\gamma}_l = \lim_{k \rightarrow 0} \gamma_l(k).$$

Moreover, we assume for the moment that  $a\hat{\gamma}_l \neq -(l+1)$ . Thus we deduce from the relation (4.121) that the phase shifts tend to zero (modulo  $\pi$ ) as  $k^{2l+1}$ . The  $S$  matrix elements (4.50) are then given by

$$S_l(k) \rightarrow 1 + 2i\bar{c}_l k^{2l+1} \quad (4.123)$$

where the constants  $\bar{c}_l$  are real numbers. Similarly, the partial wave amplitudes (4.65), which are proportional to  $\delta_l/k$  for small  $k$ , exhibit the low energy behaviour

$$a_l(k) \rightarrow \bar{c}_l k^{2l}. \quad (4.124)$$

Except for the s-wave ( $l=0$ ) contribution which in general tends towards a non-zero constant, all partial cross sections  $\sigma_l$  ( $l \geq 1$ ) vanish as  $k^{4l}$ . The scattering is therefore *isotropic* at very low energies and  $\sigma_{\text{tot}} = \sigma_0$ . It is convenient to define the *scattering length*  $\alpha$  as [29]

$$\alpha = - \lim_{k \rightarrow 0} \frac{\tan \delta_0(k)}{k}. \quad (4.125)$$

We shall study in Section 11.6 various properties of the scattering length within the context of the effective range theory. For the moment, we note that as  $k \rightarrow 0$  the  $s$ -wave partial amplitude is given by [30]

$$\lim_{k \rightarrow 0} a_0(k) = \lim_{k \rightarrow 0} \frac{\sin \delta_0(k)}{k} = -\alpha \quad (4.126)$$

so that the scattering amplitude (4.66) is such that

$$f \xrightarrow{k \rightarrow 0} -\alpha. \quad (4.127)$$

Hence the differential scattering cross section becomes

$$\frac{d\sigma}{d\Omega} \xrightarrow{k \rightarrow 0} \alpha^2 \quad (4.128)$$

and

$$\sigma_{\text{tot}} \xrightarrow{k \rightarrow 0} 4\pi\alpha^2. \quad (4.129)$$

If by accident

$$a\hat{\gamma}_l = -(l+1) \quad (4.130)$$

the above conclusions are modified. Let us first examine the case  $l > 0$ . Then, by using eqs. (4.117) and (4.130) we see that

$$q_l \xrightarrow{k \rightarrow 0} -\frac{l}{l+1} + \mathcal{O}(k^2 a^2), \quad > 0. \quad (4.131)$$

Thus, inserting eq. (4.131) into eq. (4.115), we deduce that as  $k \rightarrow 0$  the quantity  $\tan \delta_l$  now behaves as  $k^{2l-1}$  and the  $S$ -matrix elements are such that

$$S_l(k) \xrightarrow{k \rightarrow 0} 1 + 2i\bar{d}_l k^{2l-1}, \quad l > 0 \quad (4.132)$$

where the constants  $\bar{d}_l$  are real. The corresponding partial wave amplitudes are given by

$$a_l(k) \xrightarrow{k \rightarrow 0} \bar{d}_l k^{2l-2}, \quad l > 0. \quad (4.133)$$

As a consequence, if  $a\hat{\gamma}_1 = -2$ , so that the anomalous behaviour occurs in the p-wave ( $l = 1$ ), the scattering amplitude (4.66) is given as  $k \rightarrow 0$  by

$$f \xrightarrow{k \rightarrow 0} -\alpha + \beta \cos \theta \quad (4.134)$$

where  $\alpha$  is the scattering length (4.125) and  $\beta$  is a constant. Hence the differential cross section is never isotropic in that case, even when  $k = 0$ . On the contrary, if eq. (4.130) holds for  $l \geq 2$ , we see that the relation (4.133) implies that the results (4.127)–(4.129) are unchanged.

The case  $l = 0$  requires special consideration. Indeed, if  $a\hat{\gamma}_0 = -1$ , we deduce from eq. (4.119) that

$$q_0 \xrightarrow{k \rightarrow 0} \frac{1}{3}(ka)^2 + \mathcal{O}(k^4 a^4), \quad l = 0. \quad (4.135)$$

Therefore, using eq. (4.118), we see that when  $k$  tends to zero, the quantity  $\tan \delta_l$  behaves as  $k^{-1}$ , so that the phase shift  $\delta_0$  reaches the value  $\frac{1}{2}\pi$  (modulo  $\pi$ ). Hence in this case the  $S$ -matrix element  $S_0$  and s-wave amplitude  $a_0(k)$  are such that

$$S_0(k) \xrightarrow{k \rightarrow 0} -1; \quad a_0(k) \underset{k \rightarrow 0}{\sim} i/k. \quad (4.136)$$

We note that the scattering length  $\alpha$  is such that  $\alpha \rightarrow \infty$  when  $k \rightarrow 0$ . More precisely, by using the definition (4.125) together with the fact that  $\tan \delta_l \sim k^{-1}$  as  $k \rightarrow 0$ , we see that  $\alpha$  diverges like  $k^{-2}$  when  $k$  tends to zero. Moreover, the relation (4.126) breaks down, the scattering amplitude is given by  $f \sim i/k$  and the total cross section is such that

$$\sigma_{\text{tot}} \xrightarrow{k \rightarrow 0} \infty \quad \text{as} \quad k^{-2} \text{ (or } E^{-1}). \quad (4.137)$$

This singular case is often called a “zero-energy resonance”. Its physical significance will be illustrated below in the case of the scattering by a square well potential.

#### 4.3.4. Behaviour of the phase shifts for large $l$

We have already pointed out that an increase in the value of  $l$  (for fixed  $k$ ) tends to diminish the importance of a given potential of finite range because of the centrifugal barrier term  $l(l+1)/r^2$  appearing in the radial equation (4.17). Thus we expect that the phase shifts  $\delta_l(k)$  will tend to zero (modulo  $\pi$ )



as  $l \rightarrow \infty$  (for fixed  $k$ ). More precisely, we may return to eqs. (4.115) and (4.117) valid for  $l \gg ka$  and write the relation

$$\tan \delta_l(k) \underset{l \rightarrow \infty}{\sim} \frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \frac{l - a\gamma_l(k)}{l + 1 + a\gamma_l(k)} \quad (4.138)$$

valid for a potential of finite "range"  $a$ . This expression may be used to analyze the convergence of the partial wave series.

Another way of investigating the behaviour of the phase shifts for  $l \gg ka$  is to use the integral representation (4.106). Indeed, for a potential of finite "range", we have already shown above that the radial function  $R_l$  will differ little from the corresponding free wave  $j_l$  when  $l \gg ka$ . Hence we may write

$$\tan \delta_l \simeq (\tan \delta_l)_{B1} = -k \int_0^\infty [j_l(kr)]^2 U(r) r^2 dr, \quad l \gg ka. \quad (4.139)$$

The quantity  $(\tan \delta_l)_{B1}$  is called the *first Born approximation* [31] to  $\tan \delta_l$ . If the potential has a strict finite range, we may use the approximate formula (C.11a) for  $j_l$  to obtain the simple estimate

$$\tan \delta_l \underset{l \gg ka}{\simeq} - \frac{k^{2l+1}}{[(2l+1)!!]^2} \int_0^\infty r^{2l+2} U(r) dr. \quad (4.140)$$

For example, in the case of a square well (reduced) potential  $U(r)$  such that

$$U(r) = \begin{cases} -U_0, & r < a \\ 0, & r > a \end{cases} \quad (4.141)$$

we deduce from eq. (4.140) that

$$\tan \delta_l \underset{l \gg ka}{\simeq} U_0 a^2 \frac{(ka)^{2l+1}}{[(2l+1)!!]^2 (2l+3)}. \quad (4.142)$$

Hence, for  $l \gg ka$  (with  $k$  fixed) the quantities  $\tan \delta_l$  fall off rapidly as  $l$  increases. In fact, we have

$$\delta_{l+1}/\delta_l \simeq (ka/2l)^2, \quad l \gg ka. \quad (4.143)$$

It is worth noting that the simple formula (4.140) cannot be used for interaction potentials which have a sizable "tail", since the major contribution to the integral (4.139) then comes from the region near the point  $r_0 = l/k$  where the function  $j_l(kr)$  takes on significant values. This is the case in particular for the Yukawa potential

$$U(r) = U_0 e^{-r/a}/r, \quad (4.144)$$

and for potentials having the form  $U_0/r^s$  at large  $r$ .

#### 4.3.5. The phase shifts at high energies

Let us now investigate the behaviour of the phase shifts when  $l$  is fixed but  $k \rightarrow \infty$ . In this case we expect from eq. (4.17) that the importance of the potential will become vanishingly small so that the radial function  $R_l$  will

again be very close to the corresponding free wave. Thus, using the first Born approximation expression (4.139), and with the help of the asymptotic expression (C.12a), we deduce that [32–33]

$$\tan \delta_l \xrightarrow[k \rightarrow \infty]{} -\frac{1}{2}k^{-1} \int_0^\infty U(r) dr + \mathcal{O}(k^{-2}). \quad (4.145)$$

Hence we see that the phase shifts  $\delta_l(k)$  tend to zero (modulo  $\pi$ ) as  $k \rightarrow \infty$ . This suggests that a reasonable *absolute* definition of phase shifts may be given by requiring that

$$\lim_{k \rightarrow \infty} \delta_l(k) = 0. \quad (4.146)$$

We note that this definition is physically very similar to that discussed after eq. (4.107), since in both cases we require that  $\delta_l = 0$  when the particle is effectively free.

## 4.4. Examples

In this section we shall illustrate the method of partial waves on two simple examples: the square well and the hard sphere potentials.

### 4.4.1. Scattering by a square well

Let us first consider an attractive square well potential such that

$$U(r) = \begin{cases} -U_0 & (U_0 > 0), & r < a \\ 0, & r > a \end{cases} \quad (4.147)$$

which is illustrated on Fig. 4.5. For  $r < a$ , the radial equation (4.17) becomes

$$[d^2/dr^2 + \kappa^2 - l(l+1)/r^2]u_l(r) = 0, \quad r < a \quad (4.148)$$

where we have set

$$\kappa = \sqrt{k^2 + U_0} \quad (4.149)$$

and we do not write out explicitly the  $k$ -dependence of  $u_l$  in order to simplify the notation. The regular solution of eq. (4.148) is given by

$$u_l(r) = C_l r j_l(\kappa r), \quad r < a \quad (4.150)$$

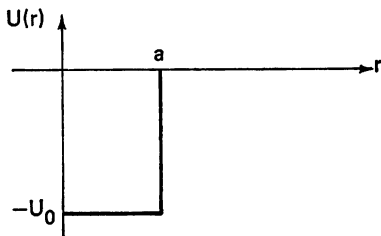


Fig. 4.5. The attractive square well of the text.

where  $C_l$  is independent of the variable  $r$ . Hence the “interior” radial wave function  $R_l(r)$  is given by

$$R_l(r) = C_l j_l(\kappa r), \quad r < a. \quad (4.151)$$

In the region  $r > a$ , where there is no interaction, the “exterior” radial function, normalized for example according to eq. (4.86b) is such that

$$R_l(r) = j_l(\kappa r) - \tan \delta_l n_l(\kappa r). \quad (4.152)$$

Therefore, by matching the two functions (4.151) and (4.152) together with their first derivatives at  $r = a$ , we find that the quantity  $\tan \delta_l$  is given by eq. (4.113a), with

$$\gamma_l = \kappa j'_l(\kappa a)/j_l(\kappa a). \quad (4.153)$$

Let us first consider s-wave scattering. Thus, for  $l = 0$  we use the fact that  $j_0(x) = (\sin x)/x$  and  $n_0(x) = -(\cos x)/x$  to deduce from eqs. (4.113a) and (4.153) that

$$\tan \delta_0 = \frac{k \tan(\kappa a) - \kappa \tan(ka)}{\kappa + k \tan(ka) \tan(\kappa a)} \quad (4.154)$$

or

$$\delta_0 = -ka + \tan^{-1} \left[ \frac{k}{\kappa} \tan \kappa a \right]. \quad (4.155)$$

The behaviour of  $\delta_0$  at low energies ( $ka \ll 1$ ) is of particular interest. Let us first assume that the potential is *weak*, so that  $U_0 a^2 \ll 1$ . In this case we note from eq. (4.149) that we also have  $\kappa a \ll 1$ . Hence, if we require that  $\delta_0 \rightarrow 0$  when  $U_0 \rightarrow 0$  (according to the absolute definition of phase shifts given on p. 79), we infer from eq. (4.155) that  $\delta_0 \rightarrow 0$  as  $k \rightarrow 0$ . For finite values of  $k$  such that  $ka \ll 1$  we have approximately

$$\delta_0 \simeq ka \left[ \frac{\tan \kappa a}{\kappa a} - 1 \right]. \quad (4.156)$$

We also note that the scattering length (4.125) is given by

$$\alpha = \left[ 1 - \frac{\tan \lambda_0 a}{\lambda_0 a} \right] a \quad (4.157)$$

with  $\lambda_0 = \sqrt{U_0}$ . Therefore, since  $\lambda_0 a \ll 1$  for a weak interaction, we see from eq. (4.157) that  $\alpha$  is negative in this case, while the s-wave cross section is finite and given by  $\sigma_0 = 4\pi\alpha^2$ .

While we remain at low energies, let us increase the coupling strength  $U_0$  so that (for fixed  $k$ ) the quantity  $\kappa a$  also becomes bigger. We see that as  $\kappa a$  increases from zero to  $\frac{1}{2}\pi$ ,  $\delta_0$  grows from zero to about  $\frac{1}{2}\pi$ . In particular, at zero energy we have  $\kappa a = \lambda_0 a$  and we find that when  $\lambda_0 a = \frac{1}{2}\pi$  (or  $U_0 a^2 = \frac{1}{4}\pi^2$ ) the zero-energy phase shift is given by

$$\lim_{k \rightarrow 0} \delta_0(k) = \frac{1}{2}\pi. \quad (4.158)$$

In this case the scattering length (4.157) becomes infinite and the s-wave cross section  $\sigma_0$  diverges like  $k^{-2}$  at  $k = 0$ : this is a “zero energy resonance” as described at the end of Section 4.3.3.

This anomalous behaviour is directly connected with the existence of an s-wave bound state in the potential well. Indeed, if there is such a bound state at an energy  $E_0 < 0$ , then the “exterior” wave function for  $r > a$  has the form

$$R_0^B(r) = N_0 r^{-1} \exp(-k_0 r), \quad r > a \quad (4.159)$$

where the superscript B indicates that it is a *bound state* wave function,  $N_0$  is a normalization constant and we have set  $k_0^2 = -2mE_0/\hbar^2$ . The corresponding “interior” wave function is then given by eq. (4.151), in which the quantity  $\kappa$  is now replaced by  $\kappa_0 = \sqrt{U_0 - k_0^2}$ . Upon joining the interior and exterior solutions and their first derivatives at  $r = a$ , we find that  $k_0$  is determined by the roots of the equation [34]

$$\xi_0 \cot \xi_0 = -\eta_0 \quad (4.160)$$

with

$$\xi_0 = \kappa_0 a \quad \text{and} \quad \eta_0 = k_0 a. \quad (4.161)$$

When the interaction is weak so that  $\lambda_0 a < \frac{1}{2}\pi$ , eq. (4.160) cannot be satisfied and there is no s-wave bound state. In this case we have seen above that  $\delta_0$  tends to zero as  $k \rightarrow 0$ , while  $\alpha$  remains finite and negative. Now, if

$$\frac{1}{2}\pi < \lambda_0 a < \frac{3}{2}\pi \quad (4.162)$$

then eq. (4.160) can be satisfied by just *one* value of  $k_0$  so that the potential can support one s-wave bound state. The critical value  $\lambda_0 a = \frac{1}{2}\pi$  (or  $U_0 a^2 = \frac{1}{4}\pi^2$ ) at which  $\delta_0(k = 0) = \frac{1}{2}\pi$  and  $\alpha$  is infinite therefore corresponds precisely to the transition between these two regimes, i.e. to a potential which is nearly able to bind an s-state. In this case one usually says that there is a *virtual* state.

Let us now assume that  $\lambda_0 a$  satisfies the inequalities (4.162). In particular, if  $\lambda_0 a$  is just above  $\frac{1}{2}\pi$ , the phase shift  $\delta_0$  goes through  $\frac{1}{2}\pi$  and one has (see Fig. 4.6)

$$\lim_{k \rightarrow 0} \delta_0(k) = \pi. \quad (4.163)$$

Moreover, we see from eq. (4.154) and the foregoing discussion that

$$\delta_0 \simeq \pi - ka\{1 - (\tan \kappa a)/\kappa a\}. \quad (4.164)$$

By repeating the arguments made above, it is possible to show that if  $U_0$  (or  $\lambda_0$ ) is increased in such a way that the potential can support  $n$  bound s-states, then the zero-energy s-wave phase shift is such that

$$\lim_{k \rightarrow 0} \delta_0(k) = n\pi. \quad (4.165)$$

Moreover, when  $\lambda_0 a = \frac{1}{2}(2n + 1)\pi$  so that the potential is about to support its  $(n + 1)$ th bound state, we have

$$\lim_{k \rightarrow 0} \delta_0(k) = (n + \frac{1}{2})\pi. \quad (4.166)$$

The results (4.165)–(4.166) are in fact true for more general interactions than the square well considered here. As we shall see in Section 11.3 they are an example of *Levinson's theorem* [21].

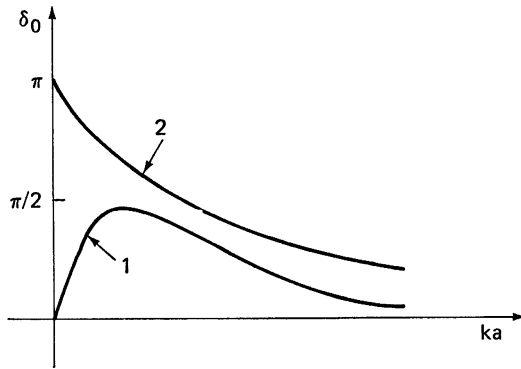


Fig. 4.6. The low-energy behaviour of the s-wave phase shift. Curve 1 corresponds to a potential which cannot support a bound state; curve 2 refers to a potential which can produce one loosely bound state.

So far we have studied the behaviour of the phase shift  $\delta_0$  at low energies as a function of the coupling strength  $U_0$ . We may also study  $\delta_0$  as a function of  $k$  for fixed values of  $U_0$  (or  $\lambda_0$ ). For example, if  $\lambda_0 a < \frac{1}{2}\pi$  so that the potential does not support a bound state, we see from eqs. (4.155) and (4.156) that at low energies, and as  $ka$  increases, the phase shift  $\delta_0$  first grows towards a value close to  $\frac{1}{2}\pi$  and then turns over and decreases. This is illustrated on Fig. 4.6, where we also display the low-energy behaviour of a phase shift  $\delta_0$  corresponding to a square well that can support a loosely bound state. In general, as  $ka$  increases, the phase shift  $\delta_0$  rises from its threshold value  $\delta_0(k = 0) = n\pi$  to a maximum which is close to  $(n + \frac{1}{2})\pi$ .

Let us further increase  $ka$  and leave the region of low energies. Then, if we require that the phase shift be a continuous function of  $k$ , we see from eq. (4.155) that  $\delta_0$  will decrease progressively from its maximum value  $\delta_0^{\max} \simeq (n + \frac{1}{2})\pi$  so that ultimately

$$\lim_{k \rightarrow \infty} \delta_0(k) = 0. \quad (4.167)$$

We now consider the *higher angular momenta* ( $l > 0$ ) and begin by analyzing the low energy region. Following the general discussion of section 4.3.3, we see that  $\tan \delta_l$  is given by eq. (4.115) for  $ka \ll l$ . Moreover, since

$\gamma_l$  is now given explicitly by eq. (4.153), we may use the relation (C.10a) of Appendix C to expand  $\gamma_l$  about  $k = 0$  as

$$\gamma_l(k) = \hat{\gamma}_l + \mathcal{O}(k^2 a^2) \quad (4.168)$$

with

$$\hat{\gamma}_l = \lim_{k \rightarrow 0} \gamma_l(k) = \lambda_0 j'_l(\lambda_0 a) / j_l(\lambda_0 a). \quad (4.169)$$

Hence the quantity  $q_l(k)$  of eq. (4.117) becomes

$$q_l(k) = [a\hat{\gamma}_l]^{-1} [l + \mathcal{O}(k^2 a^2)], \quad l > 0 \quad (4.170)$$

and we may write eq. (4.115) in the form of eq. (4.121), namely

$$\tan \delta_l(k) \simeq \frac{(ka)^{2l+1}}{ka \ll l} \frac{l - a\hat{\gamma}_l + \mathcal{O}(k^2 a^2)}{(2l+1)!!(2l-1)!! l + 1 + a\hat{\gamma}_l + \mathcal{O}(k^2 a^2)} \quad (4.171)$$

where  $\hat{\gamma}_l$  is given by eq. (4.169).

It is apparent from eq. (4.171) that at low energies none of the phase shifts with  $l > 0$  contribute much to the scattering in comparison with the s-wave phase shift (4.155), except when the denominator in eq. (4.171) vanishes. In this case we see that  $\delta_l$  passes through  $\frac{1}{2}\pi$  (modulo  $\pi$ ) and the partial-wave cross section  $\sigma_l$  reaches its maximum value (4.73). This behaviour corresponds to a *resonance* and will be analyzed in more detail in Section 4.5. We already note here that a *necessary* condition for a resonance to appear at low energies is that

$$|a\hat{\gamma}_l + l + 1| \ll 1. \quad (4.172)$$

With the help of eq. (4.169) and the recursion relation (C.13c) of Appendix C, we may rewrite this condition as

$$|\lambda_0 a j_{l-1}(\lambda_0 a) / j_l(\lambda_0 a)| \ll 1. \quad (4.173)$$

We now recall that the condition

$$j_{l-1}(\lambda_0 a) = 0 \quad (4.174)$$

corresponds precisely to the appearance of a bound state with zero energy for a particular  $l$ -value [35]. Thus, we deduce from eq. (4.171) that if we impose the condition  $\delta_l \rightarrow 0$  as  $U \rightarrow 0$ , then we have  $\delta_l \rightarrow 0$  as  $k \rightarrow 0$  for a potential which cannot support a bound state of angular momentum  $l$ . As we increase the coupling strength and reach the first non-zero value of  $\lambda_0 a$  such that the condition (4.174) is satisfied [i.e. a potential which can just support *one* bound-state of angular momentum  $l$ ] we see from eq. (4.171) that  $\delta_l \rightarrow \pi$  as  $k \rightarrow 0$ . By repeating this argument we verify the Levinson theorem [21] (see also Section 11.3), namely

$$\lim_{k \rightarrow 0} \delta_l(k) = n_l \pi \quad (4.175)$$

where  $n_l$  is the number of bound states of angular momentum  $l > 0$  which can be supported by the potential. We note that in contrast to the s-wave case, and

because of the factor  $(ka)^{2l+1}$  appearing in the numerator of eq. (4.171), the “anomalous” behaviour (4.166) cannot happen for  $l > 0$ .

We may also deduce from the above discussion the low-energy behaviour of the phase shift  $\delta_l$  as a function of  $k$ . If the potential cannot support a bound state of angular momentum  $l$ , and is very weak, then the phase shift  $\delta_l$  will quickly turn over and decrease (see curve 1 of Fig. 4.7). If the potential is almost attractive enough to support a bound state in the  $l$ -wave, then the phase shift will exhibit the behaviour shown by the curve 2. We also display in Fig. 4.7 the low-energy behaviour of a phase shift which corresponds to a potential producing one loosely bound state of angular momentum  $l$  (curve 3).

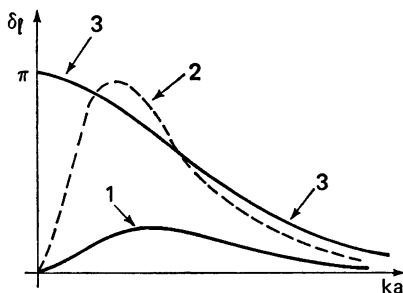


Fig. 4.7. The low-energy behaviour of a phase shift  $\delta_l$  for  $l > 0$ . Curve 1 corresponds to a very weak potential, curve 2 to a potential which nearly supports one bound state of angular momentum  $l$  and curve 3 to a potential which can produce one loosely bound state having the angular momentum  $l$ .

Let us now consider the phase shifts  $\delta_l$  at high energies, for which  $ka \gg l$ . In this case we can use the asymptotic forms (C.12a) and (C.12b) to deduce from eqs. (4.113a) and (4.153) that

$$\delta_l(k) \underset{ka \gg l}{\simeq} - (ka - \frac{1}{2}l\pi) + \tan^{-1} \left[ \frac{k}{\kappa} \tan(\kappa a - \frac{1}{2}l\pi) \right]. \quad (4.176)$$

Hence, if we require that the phase shift be a continuous function of  $k$ , we see from eq. (4.176) that for  $ka \gg l$  the quantity  $\delta_l$  will decrease continuously as  $k$  increases [36] until

$$\lim_{k \rightarrow \infty} \delta_l(k) = 0. \quad (4.177)$$

We have considered thus far the case of an *attractive* square well potential. The theory of a *repulsive* square well can be developed in a similar way and is left as an exercise for the reader (see Problem II, 7).

#### 4.4.2. Hard sphere scattering

As a second example we consider the “hard sphere” potential

$$U(r) = \begin{cases} +\infty, & r < a \\ 0, & r > a. \end{cases} \quad (4.178)$$

The boundary condition in this case is particularly simple: the “exterior” wave function (4.110) must vanish at  $r = a$ , so that

$$\tan \delta_l = j_l(ka)/n_l(ka) \quad (4.179)$$

and  $\gamma_l$  is infinite.

In the low-energy limit ( $ka \ll 1$ ), the formulae (C.11) of Appendix C yield

$$\tan \delta_l \simeq - \frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \quad (4.180)$$

so that  $|\tan \delta_l|$  decreases rapidly for increasing  $l$ . We see from eq. (4.180) that in this case the low-energy scattering is *always* dominated by the  $l = 0$  partial wave, the corresponding phase shift being given by

$$\delta_0 = -ka. \quad (4.181)$$

In the limit  $k \rightarrow 0$  all the phase shifts vanish and only the s-wave contributes to the scattering amplitude (4.66). The scattering length (4.125) is given by  $\alpha = a$ . Moreover, the differential cross section at zero energy is such that

$$\frac{d\sigma}{d\Omega} \xrightarrow{k \rightarrow 0} a^2 \quad (4.182)$$

while the zero-energy total cross section becomes

$$\sigma_{\text{tot}} \xrightarrow{k \rightarrow 0} 4\pi a^2 \quad (4.183)$$

which is four times the classical value  $\pi a^2$ .

At high energies ( $ka \gg l$ ), we may use the asymptotic forms (C.12) of the functions  $j_l$  and  $n_l$  to obtain from eq. (4.179) the approximate expressions of the phase shifts, namely

$$\delta_l \simeq -ka + \frac{1}{2}l\pi. \quad (4.184)$$

We note that  $\delta_l \rightarrow -\infty$  as  $k \rightarrow \infty$  so that the Levinson theorem does not apply in this case. Using eqs. (4.71) and (4.184) it is possible to obtain the leading term of the total cross section in the following way. We first write

$$\sigma_{\text{tot}} \simeq \frac{4\pi}{k^2} \sum_{l=0}^{l_{\text{max}}} (2l+1) \sin^2(\frac{1}{2}l\pi - ka) \quad (4.185)$$

and remember that  $l_{\text{max}} \simeq ka$  [see Section 4.1]. Therefore, by considering successive pairs of terms in the sum on  $l$ , we have

$$\begin{aligned} \sigma_{\text{tot}} \simeq \frac{4\pi}{k^2} \{ & [\sin^2(ka) + \sin^2(ka - \frac{1}{2}\pi)] \\ & + 2[\sin^2(ka - \frac{1}{2}\pi) + \sin^2(ka - \pi)] + \cdots \} \end{aligned}$$



so that

$$\sigma_{\text{tot}} \simeq \frac{4\pi}{k^2} \sum_{l=0}^{l_{\text{max}}} l = 2\pi a^2. \quad (4.186)$$

We see from eq. (4.186) that the total cross section is twice the classical value. At first sight this result may seem surprising, because when  $ka \gg 1$  it should be possible to construct wave packets which are small by comparison with the size of the scattering region. However, because the potential exhibits a sudden discontinuity at  $r = a$  the scattering can never be treated classically. In fact, a detailed study of the differential cross section in the high energy limit shows that [e.g. 37]

$$\frac{d\sigma}{d\Omega} \simeq \frac{1}{4}a^2[1 + \cot^2(\frac{1}{2}\theta)J_1^2(ka \sin \theta)]. \quad (4.187)$$

Here  $J_1$  is a Bessel function of order one. For small  $x$  one has  $J_1(x) \simeq \frac{1}{2}x$  while for large  $x$ ,  $J_1(x) \simeq (2/\pi x)^{1/2} \cos(x - \frac{3}{4}\pi)$ . We note that the first term on the right of eq. (4.187), which is isotropic, yields precisely the classical differential cross section  $\frac{1}{4}a^2$ . The second term, which is sharply peaked in the forward direction describes the “diffraction” or “shadow” scattering produced by interference between the incident wave and the outgoing scattered wave (see Section 3.4). Thus, returning to eq. (4.186), we see that at high energies half the total cross section arises from “classical” or “reflection” scattering, while the other half is due to “diffraction” scattering.

We have considered above two simple examples for which the Schrödinger radial equation (4.17) may be solved in terms of known functions. This is also the case for the Coulomb potential, which we shall study in Chapter 6. We mention here that other interactions exist for which explicit solutions may be found, at least for some values of  $l$ . For example, the s-wave radial equation may be solved for an attractive exponential potential [38] of the form

$$U(r) = -U_0 e^{-r/a}, \quad U_0 > 0. \quad (4.188)$$

For other potentials such that the radial Schrödinger equation is solvable we refer the reader to the references [39–45] listed at the end of this chapter.

## 4.5. Resonances

### 4.5.1. Preliminaries

In general the phase shifts – and therefore the cross sections – are slowly varying functions of the incident bombarding energy and of the strength of the potential. However, under certain circumstances it may happen that a phase shift  $\delta_l$  suffers a rapid variation for a given potential strength and in a certain energy interval. The corresponding partial wave amplitude  $a_l$  and cross section  $\sigma_l$  will then change dramatically in that energy range.

Before we analyze this phenomenon, let us first recast the expression of the  $S$ -matrix element  $S_l = \exp(2i\delta_l)$  and that of the partial wave amplitude  $a_l$  in a different form. Using eq. (4.113a) we may write

$$S_l = \exp(2i\delta_l) = \exp(2i\xi_l) \frac{\gamma_l - r_l + is_l}{\gamma_l - r_l - is_l} \quad (4.189)$$

where  $\gamma_l$  is the logarithmic derivative of the interior solution at  $r = a$  and the real quantities  $\xi_l$ ,  $r_l$  and  $s_l$  are defined by the relations

$$\exp(2i\xi_l) = -h_l^{(2)}(ka)/h_l^{(1)}(ka), \quad (4.190)$$

$$r_l = \text{Re}[kh_l^{(1)'}(ka)/h_l^{(1)}(ka)] \quad (4.191)$$

and

$$s_l = \text{Im}[kh_l^{(1)'}(ka)/h_l^{(1)}(ka)]. \quad (4.192)$$

We have introduced here the spherical Hankel functions  $h_l^{(1)}$  and  $h_l^{(2)}$  [see Appendix C] together with  $h_l^{(1)'}(ka) = [dh_l^{(1)}(x)/dx]_{x=ka}$ . We note that the quantity  $(\gamma_l - r_l + is_l)/(\gamma_l - r_l - is_l)$  is of modulus one and thus can be written as  $\exp(2i\rho_l)$  where

$$\rho_l = \arg(\gamma_l - r_l + is_l) = \tan^{-1}\{s_l/(\gamma_l - r_l)\}. \quad (4.193)$$

Hence the phase shift  $\delta_l$  may be decomposed as

$$\delta_l = \xi_l + \rho_l. \quad (4.194)$$

The first term  $\xi_l$  has an interesting physical interpretation. Indeed, from eq. (4.190) we deduce immediately that

$$\xi_l = \tan^{-1}\{j_l(ka)/n_l(ka)\}. \quad (4.195)$$

Hence, according to eq. (4.179), the quantity  $\xi_l$  describes "hard sphere" scattering by a potential of "range"  $a$ ; it does *not* depend on the shape and depth of the interaction potential  $V(r)$ . On the contrary, the term  $\rho_l$  clearly depends on the details of the potential through the quantity  $\gamma_l$ .

The contribution of "hard sphere scattering" can also be displayed in the partial wave amplitudes  $a_l$  given by eq. (4.65). Indeed, with the help of eq. (4.189) we may write

$$a_l = \frac{1}{2ik} \{\exp(2i\xi_l) - 1\} + \frac{1}{k} \exp(2i\xi_l) \frac{s_l}{\gamma_l - r_l - is_l} \quad (4.196)$$

or

$$a_l = \frac{1}{k} \left[ \exp(i\xi_l) \sin \xi_l + \exp(2i\xi_l) \frac{s_l}{\gamma_l - r_l - is_l} \right] \quad (4.197)$$

so that the first term in the bracket describes pure hard sphere scattering, while the second one depends on the shape and strength of the potential.

#### 4.5.2. Low-energy scattering by a strongly attractive square well

To illustrate the above discussion and show by a simple example how resonances appear, let us consider the *low-energy scattering by a deep, attractive square well*. Specifically, we shall assume that

$$ka \ll 1, \quad (4.198)$$

$$\kappa a \gg ka \quad (4.199)$$

and

$$\kappa a > l(l+1) \quad (4.200)$$

where we recall that  $\kappa = \sqrt{k^2 + U_0} = \sqrt{k^2 + \lambda_0^2}$  and we require that the inequality (4.200) be satisfied when  $l \neq 0$ . Using the fact that  $ka \ll 1$  we deduce with the help of eqs. (C.10) of Appendix C that

$$ar_l \simeq -l-1 \quad (4.201)$$

and

$$as_l \simeq (ka)^{2l-1}/[(2l-1)!!]^2, \quad l > 0 \quad (4.202a)$$

$$as_0 = 1, \quad l = 0 \quad (4.202b)$$

while the low energy “hard sphere” phase shift  $\xi_l$  is given by eq. (4.180). We note that the quantities  $\xi_l$ ,  $r_l$  and  $s_l$  are *slowly varying functions* of  $k$  in the regime  $ka \ll 1$  which we study. On the other hand, using eq. (4.153) together with the inequality (4.199) and the asymptotic formula (C.12a), we have

$$a\gamma_l = \frac{\kappa a j'_l(\kappa a)}{j_l(\kappa a)} \simeq \kappa a \cot(\kappa a - \frac{1}{2}l\pi) - 1 \quad (4.203)$$

and we see that the logarithmic derivative  $\gamma_l$  may vary rapidly as a function of  $ka$ . It has asymptotes at the values of  $ka$  for which

$$\kappa a = \sqrt{k^2 a^2 + \lambda_0^2 a^2} = \frac{1}{2}l\pi + n\pi, \quad n \text{ integer} \quad (4.204)$$

and the energy difference corresponding to neighbouring asymptotes is given by

$$D \simeq \pi \hbar^2 \lambda_0 / ma. \quad (4.205)$$

Let us now examine the behaviour of the phase shifts. We begin by considering the case  $l > 0$ . From eqs. (4.120) and (4.203) we see that

$$\tan \delta_l(k) \simeq \frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \frac{l+1 - \kappa a \cot(\kappa a - \frac{1}{2}l\pi)}{l + \kappa a \cot(\kappa a - \frac{1}{2}l\pi)}. \quad (4.206)$$

On the other hand, we have [see eq. (4.180)]

$$\tan \xi_l(k) \simeq - (ka)^{2l+1} / \{(2l+1)!!(2l-1)!!\} \quad (4.207)$$

while eqs. (4.193) and (4.201)–(4.203) yield

$$\tan \rho_l(k) \simeq \frac{(ka)^{2l+1}}{[(2l-1)!!]^2} \frac{1}{l + \kappa a \cot(\kappa a - \frac{1}{2}l\pi)} \quad (4.208)$$

and we recall that  $\delta_l = \xi_l + \rho_l$ . We see from eqs. (4.206)–(4.208) that in a small region centered about the value  $k = k_r$  such that

$$l + \kappa a \cot(\kappa a - \frac{1}{2}l\pi) = 0 \quad (4.209)$$

the two quantities  $\delta_l$  and  $\rho_l$  may vary rapidly while  $\xi_l$  remains slowly varying. In fact, if we expand the function  $\kappa a \cot(\kappa a - \frac{1}{2}l\pi)$  (or, equivalently, the logarithmic derivative  $\gamma_l$ ) about the point  $k^2 = k_r^2$ , we find that

$$\tan \rho_l = \tan(\delta_l - \xi_l) \simeq \frac{(ka)^{2l+1}}{b_l[(2l-1)!!]^2} \frac{1}{k^2 - k_r^2} \quad (4.210)$$

where

$$b_l = \frac{\partial}{\partial k^2} [\kappa a \cot(\kappa a - \frac{1}{2}l\pi)]_{k^2=k_r^2} \simeq -\frac{1}{2}a^2 \quad (4.211)$$

and we have used the inequality (4.200). Therefore we observe that *both*  $\delta_l$  and  $\rho_l$  *increase rapidly* through an odd multiple of  $\frac{1}{2}\pi$  as  $k$  moves through the value  $k_r$ . In terms of the energy  $E = \hbar^2 k^2/2m$ , we may write eq. (4.210) in the form

$$\tan(\delta_l - \xi_l) \simeq \Gamma(E)/2(E_r - E) \quad (4.212)$$

where  $E_r = \hbar^2 k_r^2/2m$  and we are considering an energy interval  $\Delta E$  centered about  $E_r$  and small enough so that we may replace in it the curve  $\gamma_l(E)$  by its tangent. Furthermore, the quantity  $\Gamma(E)$  appearing in eq. (4.212) is given by

$$\Gamma(E) = \frac{(ka)^{2l+1}}{[(2l-1)!!]^2} \left( \frac{2\hbar^2}{ma^2} \right) \quad (4.213)$$

and we observe that

$$\frac{\Gamma}{D} \simeq \frac{2}{\pi} \frac{k}{\lambda_0} \frac{(ka)^{2l}}{[(2l-1)!!]^2} \ll 1. \quad (4.214)$$

The relation (4.212) also suggests that we introduce the quantity

$$\delta_l^r = \tan^{-1} \{ \Gamma(E)/2(E_r - E) \} \quad (4.215)$$

such that in the interval  $\Delta E$  we have  $\rho_l \simeq \delta_l^r$  and

$$\delta_l \simeq \xi_l + \delta_l^r. \quad (4.216)$$

We note from eqs. (4.213) and (4.215) that  $\tan \delta_l^r$  is small and of the order of  $\Gamma(E)/2E_r$ , except in a narrow region centered about  $E = E_r$ , whose width is given approximately by the constant value  $\Gamma = \Gamma(E_r)$  [with  $\Gamma \ll \Delta E$ ]. In fact, *outside* the interval  $(E_r - \frac{1}{2}\Gamma, E_r + \frac{1}{2}\Gamma)$ , it is apparent from eqs. (4.207) and (4.208) that the phase shift  $\delta_l$  is dominated by the “hard sphere” contribution  $\xi_l$ . In that region the potential acts like a hard sphere and the incident wave does not penetrate deeply in the scattering region.

On the contrary, *within* the small energy region  $(E_r - \frac{1}{2}\Gamma, E_r + \frac{1}{2}\Gamma)$ , the quantity  $\delta_l^r$  increases rapidly through an odd multiple of  $\frac{1}{2}\pi$  and now dominates

the behaviour of the phase shift  $\delta_l$ . We also remark that near  $E = E_r$  we may write the  $S$ -matrix element (4.189) in the form

$$\exp(2i\delta_l) = \exp\{2i(\xi_l + \delta_l^0)\} = \exp(2i\xi_l) \frac{E - E_r - \frac{1}{2}i\Gamma}{E - E_r + \frac{1}{2}i\Gamma} \quad (4.217)$$

while the partial wave amplitude  $a_l$  is given by

$$a_l = \frac{1}{k} \left[ \exp(i\xi_l) \sin \xi_l + \exp(2i\xi_l) \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} \right]. \quad (4.218)$$

Since the “hard sphere” phase shift  $\xi_l$  is a smoothly varying function of the energy, it is clear that the quantity  $a_l$  will be dominated in the vicinity of  $E = E_r$  by the second term on the right of eq. (4.218). If we neglect for a moment the “hard sphere” scattering, together with the contribution of the other partial waves (we shall investigate this point in more detail below), we obtain from eqs. (4.64) and (4.218) the scattering amplitude

$$f \simeq \frac{2l+1}{k} \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} P_l(\cos \theta) \quad (4.219)$$

and the corresponding differential cross section is given by

$$\frac{d\sigma(\theta)}{d\Omega} \simeq \frac{d\sigma_l(\theta)}{d\Omega} = \frac{(2l+1)^2}{k^2} \frac{\Gamma^2}{4(E_r - E)^2 + \Gamma^2} P_l^2(\cos \theta). \quad (4.220)$$

We note that for any angle  $\theta$  the quantity  $d\sigma/d\Omega$  exhibits a *sharp peak* of width  $\Gamma$  about the value  $E = E_r$ . Moreover, in the neighbourhood of  $E_r$  the angular distribution does not depend on the energy, but only on the angular momentum  $l$  involved. This behaviour is characteristic of a *pure, narrow resonance*. Integrating eq. (4.220) over the angular variable, we obtain the *pure resonance total cross section*

$$\sigma_{\text{tot}} \simeq \sigma_l = \frac{4\pi(2l+1)}{k^2} \frac{\Gamma^2}{4(E - E_r)^2 + \Gamma^2} \quad (4.221)$$

which is known as the (one-level) *Breit-Wigner formula*. It has the characteristic *Lorentz shape* displayed in Fig. 4.8. We also note that at  $E = E_r$  the pure resonance cross section  $\sigma_l$  reaches its maximum possible value  $\sigma_l^{\text{max}} = 4\pi(2l+1)/k^2$  [see eq. (4.73)]. The energy  $E_r$  is known as the *position* and  $\Gamma$  as the *width* of the resonance.

It is obvious from the above discussion that a pure Breit-Wigner resonance represents an idealization. In particular, the width  $\Gamma$  is not strictly constant. Moreover, we have neglected a “background” contribution which consists of

- i) scattering contributed by the other partial waves ( $\neq l$ ),
- ii) “hard sphere” scattering in the partial wave  $l$ .

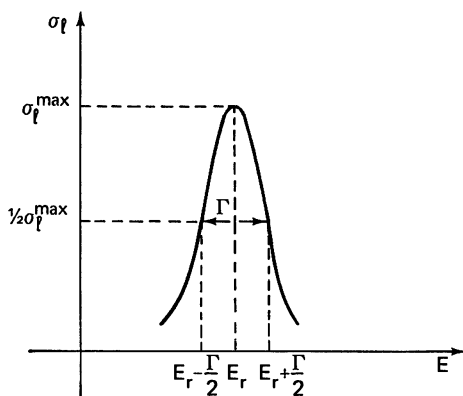


Fig. 4.8. The Lorentz shape of a pure resonance cross section.

Let us first consider the scattering from other partial waves. We shall assume that the resonances are sufficiently narrow and well separated so that only *one* resonance occurs within the energy domain under consideration. In fact, since we are studying the low-energy region ( $ka \ll 1$ ), we may estimate the contribution to the total cross section from other partial waves (which is of a pure “hard sphere” nature) to be of the order of  $4\pi a^2$  (see Section 4.4.2). This should be compared with the contribution  $4\pi(2l+1)/k^2$  of the pure  $l$ -wave resonance at  $E = E_r$  [see eq. (4.221)].

Hard sphere scattering in the partial wave  $l$  is also small in the example considered here. Furthermore, it may be taken into account by a simple modification of the above formulae. Thus, starting from eq. (4.218), we write

$$\frac{d\sigma_l(\theta)}{d\Omega} = \frac{(2l+1)^2}{k^2} \left| \exp(i\xi_l) \sin \xi_l + \exp(2i\xi_l) \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} \right|^2 P_l^2(\cos \theta), \quad (4.222)$$

so that

$$\sigma_l = \frac{4\pi(2l+1)}{k^2} \left[ \sin^2 \xi_l + \frac{\Gamma^2}{4(E - E_r)^2 + \Gamma^2} + 2 \operatorname{Re} \left( \exp(i\xi_l) \sin \xi_l \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} \right) \right]. \quad (4.223)$$

The first term on the right-hand side accounts for pure hard-sphere scattering, the second represents the pure resonance contribution, and the third term is an interference term. Since  $\xi_l$  is small in our example [see eq. (4.207)] we see that eq. (4.223) practically reduces to the pure resonance (Breit-Wigner) formula (4.221), the energy value for which  $\sigma_l$  reaches its maximum being slightly shifted from the resonance energy  $E_r$ . However, in more general circumstances it may well happen that the contribution of  $\xi_l$  could affect  $\sigma_l$  in a significant way. In particular, if  $\xi = \frac{1}{2}\pi$  (modulo  $\pi$ ) at the

resonance energy, then we have exactly  $\sigma_l = 0$  when  $E = E_r$ ! This is illustrated in Fig. 4.9, where we show in this case a typical behaviour of  $\sigma_l$  as a function of the energy.

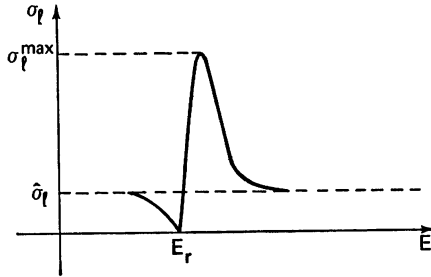


Fig. 4.9. A typical behaviour of the cross section  $\sigma_l$  when  $\xi_l = \frac{1}{2}\pi$  at  $E = E_r$ . The quantity  $\sigma_l^0$  corresponds to “hard sphere” scattering and  $\sigma_l^{\max} = 4\pi(2l+1)/k^2$ .

In order to gain further insight into the physical significance of a narrow resonance, let us come back to our example of scattering by a strongly attractive square well. If we “normalize” the radial wave  $u_l(r) = rR_l(r)$  outside the well to unit amplitude [see eq. (4.84a)], namely

$$u_l(r) = \sin(kr - \frac{1}{2}l\pi + \delta_l), \quad r \geq a \quad (4.224)$$

then we find that near  $E = E_r$  the corresponding “interior” wave function, obtained by using the continuity condition at  $r = a$  (see Section 4.4.1) is given by

$$u_l(r) \simeq \frac{(2l-1)!!}{(ka)^l} \frac{\frac{1}{2}\Gamma}{[(E - E_r)^2 + \frac{1}{4}\Gamma^2]^{1/2}} (kr) j_l(kr). \quad (4.225)$$

It is apparent from this last equation that the probability of finding the scattered particle within the well becomes large near the energy  $E = E_r$  for which a resonance appears in the  $l$ th partial wave. In fact, we see that in this case the particle is *nearly bound* in the well. From a time-dependent point of view, we should therefore expect that a resonance will correspond to a *metastable state*, whose lifetime  $\tau$  is much longer than a typical collision time. Using Heisenberg’s uncertainty relation  $\Delta E \Delta t \simeq \hbar$ , with  $\Delta E \simeq \Gamma$  and  $\Delta t \simeq \tau$ , we have

$$\tau \simeq \hbar/\Gamma. \quad (4.226)$$

So far we have studied the resonance phenomenon as a function of the wave number or energy of the incident particle, but for a fixed value of the coupling constant  $\lambda_0$ . We now recall our results of Section 4.4.1, namely that a low-energy resonance in the  $l$ th partial wave ( $l > 0$ ) appears precisely when the potential is nearly strong enough to allow a new bound state of angular momentum  $l$ .

A simple physical explanation for this fact may be given if we remember that for  $l > 0$  the “effective potential”  $U_{\text{eff}}(r) = U(r) + l(l+1)/r^2$  appearing

in the radial Schrödinger equation (4.17) contains the centrifugal barrier term  $l(l+1)/r^2$ . A typical shape of  $U_{\text{eff}}$  is shown in Fig. 4.10. If we imagine for a moment that the barrier were infinitely high, then bound states with specific positive energies (for a given value of  $\lambda_0$ ) would be allowed. Now, because the barrier has only a *finite* height, none of these former positive energy bound states will remain *genuine* bound states. Those lying at high energies (such as  $E_1$  on Fig. 4.10) will simply disappear. However, those corresponding to low energies (such as  $E_2$ ) will become *metastable* states (with a long lifetime  $\tau$ ) since it is only through the “tunnel” effect that particles can escape the well, and the penetration through the barrier is small at low

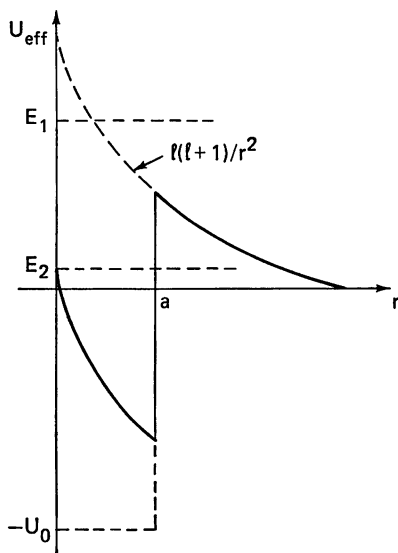


Fig. 4.10. The effective potential  $U_{\text{eff}}(r) = U(r) + l(l+1)/r^2$  (solid line) corresponding to a deep square well.

energies. We also note that as we *increase* the strength parameter  $\lambda_0$ , the resonance energies will *decrease* and move in this way towards a region where the barrier is thicker (see Fig. 4.10). We therefore expect that the lifetime  $\tau$  of these resonances will increase, so that the corresponding widths  $\Gamma$  decrease and the resonances become narrower. Eventually, if  $\lambda_0$  becomes sufficiently large, a given resonance will reach the region  $E \leq 0$  and become a *bound state*.

We now consider briefly low-energy s-wave ( $l = 0$ ) scattering by our deep square well. In this case, we have the exact relations (modulo  $\pi$ )

$$\delta_0 = \xi_0 + \rho_0, \quad (4.227)$$

$$\xi_0 = -ka \quad (4.228)$$



and

$$\rho_0 = \tan^{-1} \left( \frac{k}{\kappa} \tan \kappa a \right). \quad (4.229)$$

We note that

$$a\gamma_0 = \kappa a \cot(\kappa a) - 1. \quad (4.230)$$

Since  $ka \ll 1$  and  $\kappa \gg k$ , we may develop

$$\kappa = \sqrt{k^2 + \lambda_0^2} \simeq \lambda_0 + k^2/2\lambda_0 \quad (4.231)$$

and write

$$a\gamma_0 \simeq a\hat{\gamma}_0 + b_0 k^2 \quad (4.232)$$

with  $b_0 \simeq -\frac{1}{2}a^2$  [cf. eq. (4.211)] and

$$a\hat{\gamma}_0 = \lambda_0 a \cot(\lambda_0 a) - 1. \quad (4.233)$$

Then, using eq. (4.120), we find that

$$\tan \delta_0 \simeq -\frac{\gamma_0 k a^2}{1 + \gamma_0 a} \simeq -ka + \frac{ka \tan(\lambda_0 a)}{\lambda_0 a - \frac{1}{2}k^2 a^2 \tan(\lambda_0 a)}. \quad (4.234)$$

In accordance with the discussion of Section 4.4.1, we see that the phase shift  $\delta_0$  never increases sharply *through* an odd multiple of  $\frac{1}{2}\pi$  at low energies (see also Fig. 4.6). Moreover, in the vicinity of the  $k$ -value for which  $1 + \gamma_0 a = 0$ , the cross section

$$\sigma_0 = (4\pi/k^2) \sin^2 \delta_0 \quad (4.235)$$

is easily seen to be a monotonically decreasing function of  $ka$ . Therefore *no low-energy s-wave resonances* occur for the potential considered here [46]. This fact is easily explained by the absence of the centrifugal barrier term  $l(l+1)/r^2$  for s-waves. We note, however, that large s-wave *enhancements* in the cross sections are possible because of the “zero energy resonance” phenomenon discussed in Sections 4.3.3 and 4.4.1. We recall that this phenomenon is due to the presence of a *virtual* state (i.e., the potential is nearly strong enough to support an s-wave bound state). A well-known example of such a behaviour occurs in s-wave neutron–proton scattering in the singlet state. It is also worth pointing out that a potential  $U(r)$  which contains its own barrier is perfectly able to produce low-energy s-wave resonances.

#### 4.5.3. Resonances and time delays

Let us briefly recapitulate what we have learned from the example of Section 4.5.2. For low-energy scattering by a deep square well, and except for  $l = 0$ , there is a possibility for the phase shift  $\delta_l$  to *increase rapidly through an odd multiple of  $\frac{1}{2}\pi$  in a small energy interval* ( $E_r - \frac{1}{2}\Gamma$ ,  $E_r + \frac{1}{2}\Gamma$ ) and induce in this way a *rapid modification of the scattering amplitude and cross sections* in that energy interval. Moreover, for a pure Breit–Wigner resonance, the total cross section  $\sigma_l$  reaches its *maximum value* at the resonance energy  $E_r$ .

As we expect from the physical interpretation of resonances given above, the resonance phenomenon may happen in much more general circumstances than those described in Section 4.5.2. In fact, resonances play an important role in numerous collision processes occurring in atomic, nuclear and high-energy physics. For the case of potential scattering which we study here, resonances may appear for other interaction potentials than the square well considered above. In fact, let us return to eqs. (4.189) and (4.197) and assume that in a certain energy interval  $\Delta E$  containing the value  $E_r$  the quantities  $\xi_l$ ,  $r_l$  and  $s_l$  are nearly constant, while  $\gamma_l(E)$  may be approximated by its tangent at  $E = E_r$ , namely

$$\gamma_l(E) \simeq \gamma_l(E_r) + (E - E_r) \left[ \frac{d}{dE} \gamma_l(E) \right]_{E=E_r} \quad (4.236)$$

Then, if

$$\gamma_l(E_r) \simeq r_l \quad (4.237)$$

we see that the  $S$ -matrix element (4.189) and the partial wave amplitude (4.197) may be recast in the form of eqs. (4.217) and (4.218), respectively, with

$$\frac{1}{2}\Gamma = -s_l/B \quad (4.238)$$

and

$$B = \left[ \frac{d}{dE} \gamma_l(E) \right]_{E=E_r}. \quad (4.239)$$

Hence, in the neighbourhood of  $E = E_r$  we may write again

$$\tan(\delta_l - \xi_l) \simeq \Gamma/2(E_r - E), \quad (4.240)$$

but in the general case considered here we have no guarantee that  $\Gamma$  will be a positive quantity. If  $\Gamma$  is *positive* the quantity  $(\delta_l - \xi_l)$  will *increase* through an odd multiple of  $\frac{1}{2}\pi$  as the energy  $E$  moves through  $E_r$ ; on the contrary, if  $\Gamma$  is *negative*, then  $(\delta_l - \xi_l)$  will *decrease* through an odd multiple of  $\frac{1}{2}\pi$ .

Let us examine this point in more detail. We have shown in Section 4.3.1 that for a repulsive force corresponding to a positive (repulsive) interaction potential, the radial wave function  $R_l(r)$  is “pushed out” in comparison with the free radial wave function  $j_l(kr)$  and the phase shift  $\delta_l$  is negative. On the contrary, for an attractive potential  $\delta_l$  is positive and the radial wave function  $R_l(r)$  is “pulled in” with respect to  $j_l(kr)$  [see Fig. 4.4]. Now, it is clear that the “pushing-out” of the radial function  $R_l$  corresponds to an *advance in time*, while the “pulling in” induces a *retardation*. In the former case the scattered wave emerges from the scattering region *ahead* of the unscattered wave, while in the latter instance the scattered wave is *delayed* with respect to the free wave. In terms of the wave packet description of Section 3.5, we recall that the scattered wave packet is centered at the distance

$$r \simeq vt - [d\phi/dk]_{k=k_l} \quad (4.241)$$

where  $\phi = \arg f$  is the phase of the scattering amplitude. Thus a long delay in the emergence of the scattered wave means a sharp increase of  $\phi$  as a

function of  $k$ . On the contrary, a decrease of the function  $\phi(k)$  results from an advance in time of the scattered wave packet. The amount of this time advancement is clearly limited by *causality*, since the scattered wave cannot emerge from the scattering region before the incident wave has reached it. Hence, if  $a$  denotes the target linear dimension (which in our case may be taken as the “range” of the potential), the maximum time advancement  $\Delta t_{\max}$  is roughly given by

$$\Delta t_{\max} \simeq a/v \quad (4.242)$$

and we deduce from eq. (4.241) that

$$d\phi/dk \geq -a. \quad (4.243)$$

In particular, if the  $l$ th partial wave strongly dominates the scattering amplitude, giving a sharp peak in the vicinity of the energy  $E_r$ , the corresponding phase shift must be such that

$$d\delta_l(k)/dk \geq -a. \quad (4.244)$$

This important inequality, known as the *Wigner causality condition* [47] has important implications. In particular, we see that a phase shift may *rise quickly through* an odd multiple of  $\frac{1}{2}\pi$ , but can only *fall relatively slowly* through that quantity. Hence, returning to eq. (4.240), we remark that in the former case  $\Gamma$  is positive and may be very small; then we have a *narrow resonance* corresponding to a long *time delay*. In fact, for a pure Breit–Wigner resonance, we infer from eqs. (4.219) and (4.241) that this time delay is given by

$$\Delta t = v^{-1} \frac{d\phi}{dk} = \hbar \frac{d}{dE}(\arg f) = \hbar \frac{\frac{1}{2}\Gamma}{(E - E_r)^2 + (\frac{1}{2}\Gamma)^2} \quad (4.245)$$

and reaches its maximum value at  $E = E_r$ . On the contrary, if the phase shift decreases through an odd multiple of  $\frac{1}{2}\pi$ , then  $\Gamma$  is negative and causality imposes a lower bound on  $|\Gamma|$ . Any corresponding peak in the cross section, arising from a time advanced scattered wave, will be broad and does *not* correspond to a resonance. Thus, in accordance with the remarks of Section 4.5.2, resonances are associated with *metastable states* of lifetime  $\tau \simeq \hbar/\Gamma$  which induce a long *time delay* in the scattering. Moreover, the phase shift *increases* sharply through an odd multiple of  $\frac{1}{2}\pi$  in the neighbourhood of the resonance energy, and the partial wave amplitude exhibits a *pole* at  $E = E_r - \frac{1}{2}i\Gamma$  ( $\Gamma > 0$ ).

Finally, let us comment briefly about the *measurement* of time delays. In most experiments, one wants to obtain the variation of the cross section as a function of the incident energy. It is then necessary to work with incident particles whose energy spread  $\Delta E$  is very small. In particular, one must have

$$\Delta E \ll \Gamma. \quad (4.246)$$

In this case, however, the time  $\Delta t = \hbar/\Delta E$  required for the wave packet to enter completely into the interaction region is much longer than the lifetime

$\tau = \hbar/\Gamma$  of the resonance, so that the quantity  $\tau$  cannot be measured. In order to measure the quantity  $\tau$ , it is necessary to perform the experiment with a beam whose energy resolution  $\Delta E$  is poor and such that  $\Delta E \gg \Gamma$ .

#### 4.5.4. Resonances and Argand diagrams

Since the scattering amplitude  $f$  is a complex quantity, we may represent it for a given angle  $\theta$  and energy  $E$  (or wave number  $k$ ) by a vector (or a point) in the complex plane ( $\text{Re } f, \text{Im } f$ ), i.e. as an *Argand diagram*. We may then study the behaviour of this vector as the energy, wave number or angle are modified. Similarly, we may draw Argand diagrams for the partial wave amplitudes  $a_l$  and analyze their behaviour as  $k$  or  $E$  are modified. In fact, it will prove convenient in what follows to plot the function

$$z = 2ka_l = -i[\exp(2i\delta_l) - 1], \quad (4.247)$$

which is displayed in Fig. 4.11. We see that the point  $z$  lies on a circle of radius one and whose center is at  $+i$ .

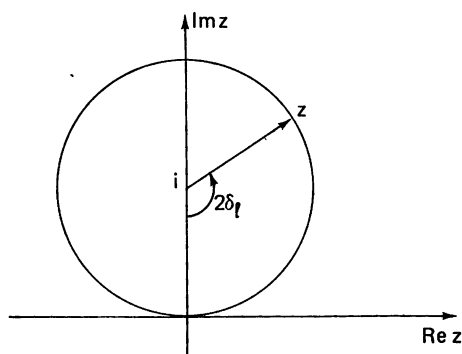


Fig. 4.11. The Argand diagram of the function  $z = 2ka_l = -i[\exp(2i\delta_l) - 1]$ .

Now, for a *pure Breit-Wigner resonance*, the phase shift  $\delta_l$  is just given by  $\delta_l = \tan^{-1}\{\Gamma/2(E_r - E)\}$  [see eq. (4.215)] and exhibits the behaviour shown on Fig. 4.12(a). In particular, we note that  $\delta_l = \frac{1}{4}\pi$  at  $E = E_r - \frac{1}{2}\Gamma$  and that  $\delta_l = \frac{3}{4}\pi$  at  $E = E_r + \frac{1}{2}\Gamma$ . Moreover, in this case the scattering amplitude may be written as

$$a_l = \frac{1}{k} \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} \quad (4.248)$$

in the vicinity of  $E = E_r$ . Thus as the energy increases, the point  $z$  will move quickly around the circle shown in Fig. 4.12(b) in an *anti-clockwise* manner. We note that the point  $E = E_r$  corresponds to the top of the circle.

In the presence of a background ("hard sphere") term, the phase shift  $\delta_l$  is given in the vicinity of the resonance energy by eq. (4.216), while  $a_l$  is obtained from eq. (4.218). Hence the points corresponding to the pure resonance case

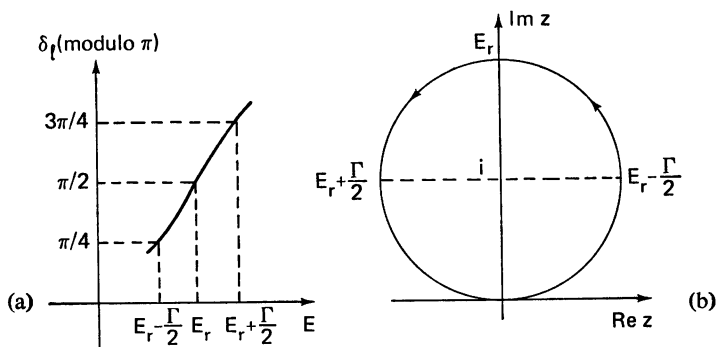


Fig. 4.12. The behaviour (a) of the phase shift  $\delta_l$  and (b) of the function  $z = -i[\exp(2i\delta_l) - 1]$  in the vicinity of the energy  $E_r$  corresponding to a pure Breit-Wigner resonance.

and lying on the upper half circle of Fig. 4.12(b) are now rotated by an angle  $2\xi_l$  and shifted by an amount  $z_1 = -i[\exp(2i\xi_l) - 1]$ . In the vicinity of the resonance energy  $E_r$ , the characteristic feature of the resonance behaviour remains a rapid *anti-clockwise* motion of the point  $z$  as the energy increases.

#### 4.6. Absorption processes. Scattering by a complex potential

We have seen in Chapter 1 that when a particle collides with a target, phenomena other than elastic scattering are in general possible. That is, there may be one, several or an infinite number of *open channels* (see Section 1.2) in addition to the elastic one. In order to take this fact into account in the partial wave method, let us return to the asymptotic behaviour (4.90a) of the scattering wave function, namely

$$\psi_{k_1}^{(+)}(k, \mathbf{r}) \rightarrow A(k) \sum_{l=0}^{\infty} (2l+1) \frac{i}{2kr} [(-1)^l e^{-ikr} - S_l e^{ikr}] P_l(\cos \theta) \quad (4.249)$$

with  $S_l = \exp(2i\delta_l)$ . We recall that this result has been obtained in Section 4.1 for the case of pure elastic scattering, such that  $\delta_l$  is real and  $|S_l| = 1$ . In order to generalize eq. (4.249) to the case where “non-elastic” processes are allowed, we remark that the interaction can only alter the *outgoing* part of the wave function. Therefore, since particles can now be removed from the incident (elastic) channel, we require that the amplitude of the outgoing radial wave be either *reduced* (if non-elastic processes occur) or left *unchanged* (if there is only elastic scattering) so that

$$|S_l| \leq 1. \quad (4.250)$$

This suggests that we introduce *complex* phase shifts

$$\delta_l = \text{Re } \delta_l + i \text{Im } \delta_l. \quad (4.251)$$

Hence we have

$$S_l = \exp(2i\delta_l) = \eta_l \exp(2i \text{Re } \delta_l) \quad (4.252)$$

where the quantity

$$\eta_l = \exp(-2 \operatorname{Im} \delta_l) \quad (4.253)$$

is often called the “inelasticity” or “absorption” factor, the term absorption being understood in the sense that particles disappear from the incident channel. Because of eq. (4.250), we have

$$0 \leq \eta_l \leq 1 \quad (4.254)$$

and

$$\operatorname{Im} \delta_l \geq 0. \quad (4.255)$$

We note that the special case  $\eta_l = 1$  (i.e.  $\operatorname{Im} \delta_l = 0$ ) corresponds to pure elastic scattering (no absorption).

The calculation of the *elastic scattering amplitude* may be done by a method entirely similar to that of Section 4.1.4. By requiring that in the elastic channel the wave function  $\psi_{k_i}^{(+)}$  should exhibit the asymptotic behaviour

$$\psi_{k_i}^{(+)} \xrightarrow{r \rightarrow \infty} A[\exp(i\mathbf{k}_i \cdot \mathbf{r}) + f_{el} e^{ikr}/r] \quad (4.256)$$

one finds from eqs. (4.249) and (4.252) that  $f_{el}$  is given by eq. (4.63) namely

$$f_{el} = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)[\exp(2i\delta_l) - 1]P_l(\cos \theta) \quad (4.257)$$

or

$$f_{el} = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)[\eta_l \exp(2i \operatorname{Re} \delta_l) - 1]P_l(\cos \theta). \quad (4.258)$$

The elastic differential cross section reads

$$\frac{d\sigma_{el}}{d\Omega} = \frac{1}{4k^2} \left| \sum_{l=0}^{\infty} (2l+1)[\eta_l \exp(2i \operatorname{Re} \delta_l) - 1]P_l(\cos \theta) \right|^2 \quad (4.259)$$

and the *total elastic* cross section is given by

$$\begin{aligned} \sigma_{tot}^{el} &= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)|\exp(2i\delta_l) - 1|^2 \\ &= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)|\eta_l \exp(2i \operatorname{Re} \delta_l) - 1|^2 = \sum_{l=0}^{\infty} \sigma_l^{el} \end{aligned} \quad (4.260)$$

where the partial elastic cross sections  $\sigma_l^{el}$  are such that

$$\sigma_l^{el} = \frac{\pi}{k^2} (2l+1)|\eta_l \exp(2i \operatorname{Re} \delta_l) - 1|^2. \quad (4.261)$$

The total number of particles which disappear from the incident channel per unit time is equal to minus the flux of the wave function (4.249) through a sphere of large radius centered at the origin. Let us write the expression (4.249) in the form

$$\psi_{k_i}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} A \left( \frac{e^{-ikr}}{r} C_{in}(k, \theta) + \frac{e^{ikr}}{r} C_{out}(k, \theta) \right) \quad (4.262)$$

with

$$C_{\text{in}}(k, \theta) = -\frac{1}{2ik} \sum_{l=0}^{\infty} (-1)^l (2l+1) P_l(\cos \theta) \quad (4.263a)$$

and

$$C_{\text{out}}(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) S_l(k) P_l(\cos \theta). \quad (4.263b)$$

Calling  $\mathbf{j}$  the probability current density corresponding to the wave function (4.249), we have from eqs. (3.30) and (4.262)–(4.263)

$$\mathbf{j} \cdot \hat{\mathbf{r}} = A^* A v \frac{1}{r^2} [|C_{\text{out}}(k, \theta)|^2 - |C_{\text{in}}(k, \theta)|^2] \quad (4.264)$$

where we have neglected terms of higher order in  $1/r$ . Now the incident flux through a unit area normal to  $\mathbf{k}_i$  is still given by eq. (3.36), namely

$$\mathbf{j}_{\text{inc}} \cdot \hat{\mathbf{k}}_i = A^* A v. \quad (4.265)$$

The total “reaction” cross section  $\sigma_{\text{tot}}^r$  corresponding to all *non-elastic* processes is therefore given by

$$\sigma_{\text{tot}}^r(k) = -\frac{1}{\mathbf{j}_{\text{inc}} \cdot \hat{\mathbf{k}}_i} \int \mathbf{j} \cdot \hat{\mathbf{r}} r^2 d\Omega \quad (4.266)$$

or

$$\sigma_{\text{tot}}^r(k) = \int [|C_{\text{in}}(k, \theta)|^2 - |C_{\text{out}}(k, \theta)|^2] d\Omega. \quad (4.267)$$

Using eqs. (4.263) together with the orthogonality property of the Legendre polynomials [eq. (B.5) of Appendix B] we then have

$$\sigma_{\text{tot}}^r = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)(1 - \eta_l^2) = \sum_{l=0}^{\infty} \sigma_l^r \quad (4.268)$$

with

$$\sigma_l^r = \frac{\pi}{k^2} (2l+1)(1 - \eta_l^2). \quad (4.269)$$

Therefore, the total (complete) cross section which includes both elastic and non-elastic processes is given by

$$\sigma_{\text{tot}} = \sigma_{\text{tot}}^{\text{el}} + \sigma_{\text{tot}}^r \quad (4.270)$$

or

$$\begin{aligned} \sigma_{\text{tot}} &= \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \{1 - \text{Re} \exp(2i\delta_l)\} \\ &= \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) [1 - \eta_l \cos(2 \text{Re} \delta_l)] = \sum_{l=0}^{\infty} \sigma_l \end{aligned} \quad (4.271)$$

with

$$\sigma_l = \frac{2\pi}{k^2} (2l+1) [1 - \eta_l \cos(2 \text{Re} \delta_l)]. \quad (4.272)$$

From eqs. (4.258) and (4.271) we remark that the *optical theorem* may be generalized to read

$$\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im } f_{\text{el}}(\theta = 0). \quad (4.273)$$

We also note that the maximum value of  $\sigma_l^{\text{el}}$  is obtained when  $\exp(2i\delta_l) = \eta_l \exp(2i \text{Re } \delta_l) = -1$ , i.e. in the absence of non-elastic processes ( $\eta_l = 1$ ). We thus have

$$\sigma_l^{\text{el}} \leq 4\pi(2l + 1)/k^2. \quad (4.274)$$

On the contrary, the maximum value of  $\sigma_l^{\text{f}}$  is reached for  $\eta_l = 0$  (maximum absorption), so that

$$\sigma_l^{\text{f}} \leq \pi(2l + 1)/k^2. \quad (4.275)$$

Finally, we see from eq. (4.272) that

$$\sigma_l \leq 4\pi(2l + 1)/k^2. \quad (4.276)$$

As we already remarked above, pure elastic scattering is possible and occurs when  $\eta_l = 1$ . However, non-elastic processes (for which  $0 \leq \eta_l < 1$ ) are always accompanied by elastic scattering, as we expect on physical grounds.

“Absorption” processes, which correspond to the removal of particles from the incident channel have led us above to introduce complex phase shifts. This notion is also directly linked to the concept of a *complex* or *optical potential*. Indeed, if we consider a potential of the type

$$V = V_{\text{R}} - iV_{\text{I}} \quad (4.277)$$

the continuity equation now takes the form

$$\nabla_{\mathbf{r}} \cdot \mathbf{j} = -\frac{2}{\hbar} V_{\text{I}} \rho \quad (4.278)$$

with  $\rho = |\psi|^2$ . Hence, for  $V_{\text{I}} > 0$ , we have a *local absorption* of the incident beam. Thus we expect that an optical potential should be able to describe elastic scattering accompanied by absorption, the latter being understood as the *sum* of all non-elastic processes [48]. We shall return to this question in Chapter 20, where a detailed study of the optical potential method will be made.

## References and notes

- [1] FAXÉN, H. and J. HOLTSMARK (1927), *Z. f. Physik* **45**, 307.
- [2] The spherical harmonics  $Y_{lm}(\theta, \phi)$  are studied in any elementary textbook on quantum mechanics. We list in Appendix B a few of their most important properties, together with those of the related Legendre polynomials  $P_l$  and associated Legendre functions  $P_l^m$ . Since there is essentially no danger of confusion with the mass  $m$  of the particle, we make use of the same (customary) symbol  $m$  to denote the magnetic quantum number.



- [3] We recall that we are considering here only the case of energies  $E \geq 0$ . For  $E < 0$  there is no acceptable solution of eq. (4.20).
- [4] MESSIAH, A. (1968), *Quantum Mechanics* (Wiley, New York) Vol. I, Chapter 9.
- [5] We shall frequently use the notation  $Y_{lm}(\hat{x})$  where  $\hat{x}$  denotes the unit vector along  $\mathbf{x}$ , and hence depends on the polar angles of  $\mathbf{x}$ .
- [6] The "range"  $a$  is here defined in a rather loose way as the distance from the origin such that the effect of the scattering potential may be neglected for values of  $r$  larger than  $a$ . For example, in the case of a Yukawa potential  $V(r) = V_0 r^{-1} \exp(-\alpha r)$ , with  $V_0 = \text{constant}$ , this "range" is given by  $a \simeq \alpha^{-1}$ . For a Coulomb potential, we see that  $\alpha \rightarrow 0$  and the concept of a "range" has no meaning since the quantity  $a$  becomes infinite.
- [7] The justification of this terminology will be given in Part III where general collision theory, based on the  $S$ -matrix concept, is studied. We shall also see in Chapter 18 that in the simple case which we consider here the  $S$ -matrix is diagonal in the angular momentum representation.
- [8] CASE, K. M. (1950), *Phys. Rev.* **80**, 797; also PAULI, W. (1933), *Handbuch der Physik* **24**, 142.
- [9] GOLDBERGER, M. L. and K. M. WATSON (1964), *Collision Theory* (Wiley, New York) Chapter 6.
- [10] It is obvious that in any physical problem the form which we assume for the interaction potential at  $r = 0$  constitutes an idealization.
- [11] INCE, E. L. (1949), *Ordinary Differential Equations* (Dover Publ., New York).
- [12] The condition (4.55) is often "derived" by requiring that the radial wave functions  $R_l = r^{-1} u_l$  [and hence the full scattering wave function  $\psi_{k_l}^{(+)}$ ] be *finite* at  $r = 0$ . However, mildly singular wave functions may be perfectly acceptable (c.f. for example the solutions of the Dirac equation for Coulomb scattering) so that the requirement of finiteness of  $R_l$  at  $r = 0$  is in fact too stringent.
- [13] MOTT, N. F. and H. S. W. MASSEY (1965), *The Theory of Atomic Collisions* (third ed., Clarendon Press, Oxford) Chapter 2.
- [14] GOLDSTEIN, H. (1957), *Classical Mechanics* (Addison-Wesley, Cambridge, Mass.) Chapter 3.
- [15] We recall that the quantity  $A(k)$  may also be chosen arbitrarily, as shown in Chapter 3.
- [16] Since we are considering functions which are not square integrable, the term "normalization" is not quite appropriate. It is however frequently used, and we shall adopt it here.

- [17] A convenient way to display this infinite variety of "normalizations" is to write

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} \cos(kr - \frac{1}{2}l\pi + \gamma) + \cot(\delta_l - \gamma) \sin(kr - \frac{1}{2}l\pi + \gamma)$$

where  $\gamma$  is a fixed constant such that

$$0 \leq \gamma < \pi.$$

[See e.g. KATO, T. (1951), *Progr. Theor. Phys.* **6**, 394.]

- [18] In order to simplify the notation we shall omit to indicate the explicit  $k$ -dependence of the quantities  $f$  and  $\delta_l$ .
- [19] The justification of this terminology will be given in Part III, where the unitarity property of the  $S$ -matrix is studied.
- [20] Other absolute definitions of phase shifts may evidently be given. We shall return to this point below [see eq. (4.146)].
- [21] LEVINSON, N. (1949), *Kgl. Danske Videnskab. Selskab. Mat.-fys. Medd.* **25**, no. 9.
- [22] It is customary to use the spectroscopic notation to describe the low partial waves. Thus the partial waves corresponding to  $l = 0, 1, 2, 3, \dots$  are called respectively the s, p, d, f,  $\dots$  waves

- [23] We present here the "standard" way of determinating the phase shifts, in which one integrates the radial equation (4.17), i.e. a *second order linear* differential equation from the origin to the asymptotic region. Another method, called the variable phase approach, consists in integrating an equivalent *first order nonlinear* differential equation. For a detailed account of this method, see for example CALOGERO, F. (1967), *Variable Phase Approach to Potential Scattering* (Academic Press, New York).
- [24] Except for the case of an infinite "wall" at  $r = a$ , where it is sufficient to require that  $R_l(r = a) = 0$ . We shall return to this question below when studying the "hard sphere" potential.
- [25] Note that the quantity  $\gamma_l$  has the dimensions of an inverse length.
- [26] Specifically, let us define the quantity  $\alpha_l = [u_l^{-1}(du_l/dr)]_{r=a}$  and introduce for convenience the functions  $s_l(x) = xj_l(x)$  and  $c_l(x) = xn_l(x)$  such that

$$s_l(x) \xrightarrow{x \rightarrow \infty} \sin(x - \frac{1}{2}l\pi)$$

and

$$c_l(x) \xrightarrow{x \rightarrow \infty} -\cos(x - \frac{1}{2}l\pi).$$

The radial function  $u_l(k, r)$  may then be written in the *exterior* region as

$$u_l(k, r) = A_l(k)[s_l(kr) \cos \delta_l - c_l(kr) \sin \delta_l]$$

and one has

$$\tan \delta_l(k) = \frac{ks'_l(ka) - \alpha_l(k)s_l(ka)}{kc'_l(ka) - \alpha_l(k)c_l(ka)} \quad (4.113')$$

where  $s'_l(ka) = [ds_l(x)/dx]_{x=ka}$  and  $c'_l(ka) = [dc_l(x)/dx]_{x=ka}$ .

- [27] This procedure is of course unnecessary if an analytic solution of the radial equation (satisfying the required boundary conditions) may be found.
- [28] If we introduce the quantities  $\beta_l(k) = [ru_l^{-1} du_l/dr]_{r=a}$  and  $\hat{\beta}_l = \lim_{k \rightarrow 0} \beta_l(k)$  we may also write eq. (4.121) as

$$\tan \delta_l \xrightarrow{k \rightarrow 0} \frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \frac{l+1-\hat{\beta}_l}{l+\hat{\beta}_l}. \quad (4.121')$$

- [29] The concept of scattering length was introduced by FERMI, E. (1936), *Ricerca Scient.* VII, 13.
- [30] We emphasize that the relations (4.126)–(4.129) only hold if  $\delta_0(k) \rightarrow 0$  (modulo  $\pi$ ) when  $k \rightarrow 0$ . We shall encounter below a particular case where this is not true [see the discussion following eq. (4.135)].
- [31] A detailed study of the first Born approximation is made in Chapter 8.
- [32] In obtaining eq. (4.145) we have also used the fact that  $\sin^2 x$  oscillates rapidly about the value  $\frac{1}{2}$  when  $x \rightarrow \infty$ .
- [33] It is clear that eq. (4.145) is only valid when the quantity  $\int_0^\infty U(r) dr$  exists.
- [34] For a detailed study of eq. (4.160), see for example SCHIFF, L. I. (1955), *Quantum Mechanics* (McGraw-Hill, New York) Section 15.
- [35] We note that when  $l > 0$  the potential strengths  $U_0$  for which the condition (4.174) is verified yield *true* zero-energy bound states. This is in contrast with the case  $l = 0$ , for which the critical potential strengths  $\lambda_0 a = \frac{1}{2}\pi, \frac{3}{2}\pi, \dots, \frac{1}{2}(2n+1)\pi$  do not yield bound states at zero energy.
- [36] Of course  $\delta_l$  must remain positive since the potential is attractive (see Section 4.3).
- [37] MORSE, P. M. and H. FESHBACH (1953), *Methods of Theoretical Physics* (McGraw-Hill, New York) Chapter 6.
- [38] BETHE H. A. and R. BACHER (1936), *Rev. Mod. Phys.* **8**, 82.
- [39] ECKART, C. (1930), *Phys. Rev.* **35**, 1303.
- [40] HULTHÉN, L. (1942), *Arkiv. Mat. Astron. Fys.* **28A**(5), **29B**(1).

- [41] BARGMANN, V. (1949), *Rev. Mod. Phys.* **21**, 488.
- [42] VOGT, E. and G. H. WANNIER (1954), *Phys. Rev.* **95**, 1190.
- [43] BHATTACHARJIE, A. and E. C. G. SUDARSHAN (1962), *Nuovo Cimento* **25**, 864.
- [44] SPECTOR, R. M. (1964), *J. Math. Phys.* **5**, 1185;  
ALY, H. H. and R. M. SPECTOR (1965), *Nuovo Cimento* **38**, 149.
- [45] NEWTON, R. G. (1966), *Scattering Theory of Waves and Particles* (McGraw-Hill, New York) Chapter 14.
- [46] In particular, the “zero energy resonance” behaviour studied at the end of Section 4.3.3 does not correspond to a genuine resonance.
- [47] WIGNER, E. P. (1955), *Phys. Rev.* **98**, 145.
- [48] The description of particular non-elastic processes is clearly beyond the scope of an optical potential approach.

# The Integral Equation of Potential Scattering

So far we have defined the stationary scattering wave function  $\psi_{\mathbf{k}_i}^{(+)}$  as a solution of the partial differential Schrödinger equation (3.19) satisfying the boundary condition (3.27). In this chapter we shall show that  $\psi_{\mathbf{k}_i}^{(+)}$  is also the solution of an equivalent *integral equation* which incorporates the boundary condition. The basic procedure is described in Section 5.1 and the necessary Green's function is evaluated in Section 5.2. The resulting integral equation for potential scattering, or *Lippmann–Schwinger equation* [1] is then obtained in Section 5.3, together with an important integral representation of the scattering amplitude. A formal, compact solution is given in Section 5.4, while the partial wave decomposition of the Lippmann–Schwinger equation is carried out in Section 5.5. We devote Section 5.6 to a mathematical analysis of the Lippmann–Schwinger equation. Finally, we consider in Section 5.7 the more general case of non-local interactions.

## 5.1. The Schrödinger equation as an integral equation

Let us rewrite the Schrödinger equation (3.19) as

$$[\nabla_{\mathbf{r}}^2 + k^2]\psi(k, \mathbf{r}) = U(\mathbf{r})\psi(k, \mathbf{r}) \quad (5.1)$$

where the right-hand side is considered as an inhomogeneous term. The general solution of this equation can be written as

$$\psi(k, \mathbf{r}) = \Phi(k, \mathbf{r}) + \int G_0(k, \mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi(k, \mathbf{r}') d\mathbf{r}' \quad (5.2)$$

where  $\Phi(k, \mathbf{r})$  is a solution of the homogeneous equation

$$[\nabla_{\mathbf{r}}^2 + k^2]\Phi(k, \mathbf{r}) = 0 \quad (5.3)$$

and where  $G_0(k, \mathbf{r}, \mathbf{r}')$  is a *Green's function* [2] corresponding to the operator  $\nabla_{\mathbf{r}}^2$  and the number  $k$ . That is,

$$[\nabla_{\mathbf{r}}^2 + k^2]G_0(k, \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'). \quad (5.4)$$

In what follows we shall simplify the notation and omit to indicate explicitly the  $k$ -dependence of the functions  $\psi$ ,  $\Phi$  and  $G_0$ .

In the scattering problem that we are considering the function  $\Phi(\mathbf{r})$  is simply the incident plane wave  $\exp(i\mathbf{k}_i \cdot \mathbf{r}) = \exp(ikz)$  with the  $z$ -axis chosen along  $\mathbf{k}_i$ . We shall denote this plane wave by  $\Phi_{\mathbf{k}_i}$  and "normalize" it in such a way that

$$\Phi_{\mathbf{k}_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}). \quad (5.5)$$

More generally, let us use Dirac's bra and ket notation and denote by

$$\Phi_{\mathbf{k}}(\mathbf{r}) \equiv \langle \mathbf{r} | \mathbf{k} \rangle = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (5.6a)$$

and

$$\Phi_{\mathbf{k}'}(\mathbf{r}) \equiv \langle \mathbf{r} | \mathbf{k}' \rangle = (2\pi)^{-3/2} \exp(i\mathbf{k}' \cdot \mathbf{r}) \quad (5.6b)$$

the plane waves corresponding to the wave vectors  $\mathbf{k}$  and  $\mathbf{k}'$  and "normalized" according to the above convention. We then have the orthogonality relation

$$\langle \Phi_{\mathbf{k}'} | \Phi_{\mathbf{k}} \rangle \equiv \langle \mathbf{k}' | \mathbf{k} \rangle = \delta(\mathbf{k} - \mathbf{k}') \quad (5.7)$$

while the closure relation reads

$$\int d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| = 1. \quad (5.8)$$

Thus, in configuration space, the (relative) probability density corresponding to this "normalization" is  $(2\pi)^{-3}$ . We note that with this choice of "normalization" the orthogonality and closure relations are very simple in momentum (or rather wave vector) space. This is in contrast with the choice  $\Phi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r})$  which corresponds to unit probability density in configuration space but leads to the relations

$$\langle \mathbf{k}' | \mathbf{k} \rangle = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') \quad (5.7')$$

and

$$(2\pi)^{-3} \int d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| = 1 \quad (5.8')$$

in wave vector space. In what follows we shall always use the "normalization" given by eq. (5.5).

Let us now return to eq. (5.2). With the function  $\Phi_{\mathbf{k}_i}(\mathbf{r})$  given by eq. (5.5), we may then write

$$\psi_{\mathbf{k}_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) + \int G_0(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k}_i}(\mathbf{r}') d\mathbf{r}' \quad (5.9)$$

where we have indicated that the function  $\psi_{\mathbf{k}_i}$  corresponds to the particular plane wave  $\Phi_{\mathbf{k}_i}$  such that  $\mathbf{k}_i$  is the incident wave vector.

## 5.2. The Green's function

We now turn to the determination of the Green's function  $G_0(\mathbf{r}, \mathbf{r}')$ . It is convenient for that purpose to work in wave vector space. Using the integral representation of the delta function

$$\delta(\mathbf{r} - \mathbf{r}') = (2\pi)^{-3} \int \exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\} d\mathbf{k}' \quad (5.10)$$

and writing [3]

$$G_0(\mathbf{r}, \mathbf{r}') = (2\pi)^{-3} \int g_0(\mathbf{k}', \mathbf{r}') \exp(i\mathbf{k}' \cdot \mathbf{r}) d\mathbf{k}' \quad (5.11)$$

we find upon substitution in eq. (5.4) that

$$g_0(\mathbf{k}', \mathbf{r}') = \exp(-i\mathbf{k}' \cdot \mathbf{r}') / (k'^2 - k^2). \quad (5.12)$$

Therefore

$$G_0(\mathbf{r}, \mathbf{r}') = - (2\pi)^{-3} \int \frac{\exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\}}{k'^2 - k^2} d\mathbf{k}'. \quad (5.13)$$

The integrand in eq. (5.13) has poles at  $k' = \pm k$ , so that we need a well defined prescription to avoid these singularities and give a meaning to the integral. We do this by invoking the boundary condition (3.27). In fact, we shall deform the integration path into the complex  $k'$  plane in such a way that  $G_0(\mathbf{r}, \mathbf{r}')$  will lead to an *outgoing spherical wave* for  $r \rightarrow \infty$ . The corresponding Green's function and stationary scattering wave will be denoted by  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  and  $\psi_{k_i}^{(+)}(\mathbf{r})$ , respectively. To see how this can be done, let us set

$$\mathbf{R} = \mathbf{r} - \mathbf{r}' \quad (5.14)$$

and choose spherical polar coordinates such that the  $z$  axis coincides with the vector  $\mathbf{R}$  (see Fig. 5.1). We then have

$$G_0(R) = - (2\pi)^{-3} \int_0^\infty dk' k'^2 \int_0^\pi d\theta' \sin \theta' \int_0^{2\pi} d\phi' \frac{\exp\{ik'R \cos \theta'\}}{k'^2 - k^2}. \quad (5.15)$$

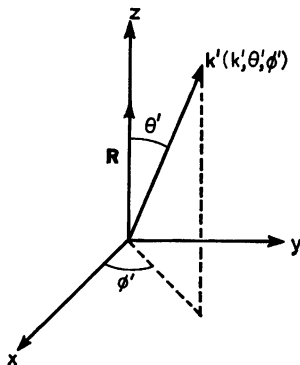


Fig. 5.1. Illustration of the vectors  $\mathbf{R}$  and  $\mathbf{k}'$  of the text.

After performing the angular integrations, we find that

$$G_0(R) = - (4\pi^2 R)^{-1} \int_{-\infty}^{+\infty} \frac{k' \sin k' R}{k'^2 - k^2} dk' \quad (5.16)$$

where we have used the fact that the integrand is an even function of  $k'$  to extend the integral on  $k'$  from  $-\infty$  to  $+\infty$ . We may also write

$$G_0(R) = - (16\pi^2 i R)^{-1} \left\{ \int_{-\infty}^{+\infty} e^{ik'R} \left[ \frac{1}{k' - k} + \frac{1}{k' + k} \right] dk' - \int_{-\infty}^{+\infty} e^{-ik'R} \left[ \frac{1}{k' - k} + \frac{1}{k' + k} \right] dk' \right\}. \quad (5.17)$$

Let us now examine the first integral

$$I_1 = \int_{-\infty}^{+\infty} e^{ik'R} \left[ \frac{1}{k' - k} + \frac{1}{k' + k} \right] dk' \quad (5.18)$$

appearing on the right-hand side of eq. (5.17). We shall analyze this expression by means of contour integration in the complex  $k'$ -plane. Thus  $k'$  becomes a complex variable

$$k' = \text{Re } k' + i \text{Im } k' \quad (5.19)$$

and

$$\exp(ik'R) = \exp(iR \text{Re } k') \exp(-R \text{Im } k'). \quad (5.20)$$

This suggests that we should write

$$I_1 = \oint_C e^{ik'R} \left[ \frac{1}{k' - k} + \frac{1}{k' + k} \right] dk' \quad (5.21)$$

and close the contour  $C$  in the upper half plane  $\text{Im } k' > 0$  by a large semi-circle  $C'$  (see Fig. 5.2), so that the contribution to the integral from this semi-circle tends to zero as we let the radius of  $C'$  tend to infinity. The integral (5.21) is then equal to its value along the real axis, for which we have four possible choices of paths  $P_1, P_2, P_3, P_4$ , as shown in Fig. 5.2.

Applying Cauchy's theorem, we then obtain for the integral  $I_1$ :

$$\begin{aligned} &\text{integrated along } P_1: 0, \\ &\text{integrated along } P_2: 2\pi i [e^{ikR} + e^{-ikR}], \\ &\text{integrated along } P_3: 2\pi i e^{-ikR}, \\ &\text{integrated along } P_4: 2\pi i e^{ikR}. \end{aligned} \quad (5.22)$$

We can proceed in the same way for the second integral

$$I_2 = \int_{-\infty}^{+\infty} e^{-ik'R} \left[ \frac{1}{k' - k} + \frac{1}{k' + k} \right] dk'. \quad (5.23)$$

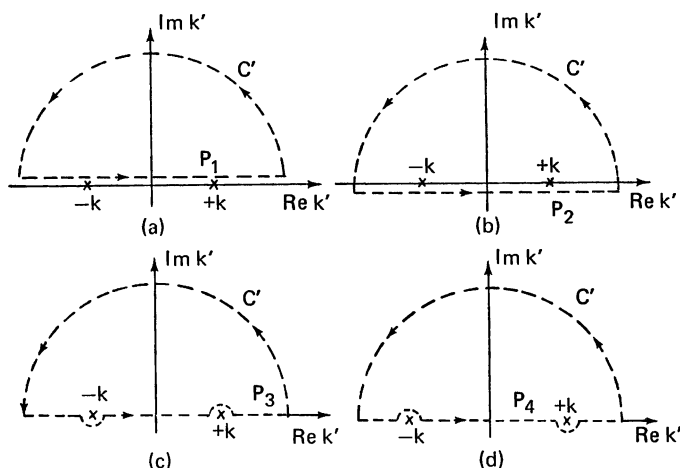


Fig. 5.2. The four possible integration contours for the evaluation of the integral  $I_1$ .

Closing now the contour in the lower-half  $k'$  plane we find for the contribution of this integral

$$\begin{aligned} \text{integrated along } P_1: & -2\pi i [e^{ikR} + e^{-ikR}], \\ \text{integrated along } P_2: & 0, \\ \text{integrated along } P_3: & -2\pi i e^{-ikR}, \\ \text{integrated along } P_4: & -2\pi i e^{ikR}. \end{aligned} \quad (5.24)$$

Therefore, we conclude that there is only *one* way of defining the Green's function  $G_0(R)$  in such a way that it behaves as a purely outgoing wave for large values of  $r$  or of  $R$ . That is,

$$G_0^{(+)}(R) = -(4\pi^2 R)^{-1} \oint_{P_4} \frac{k' \sin k'R}{k'^2 - k^2} dk' \quad (5.25)$$

so that

$$G_0^{(+)}(R) = -\frac{1}{4\pi} \frac{e^{ikR}}{R} \quad (5.26)$$

or, returning to the original variables  $\mathbf{r}$  and  $\mathbf{r}'$

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|}. \quad (5.27)$$

It is convenient to reformulate the integration prescription (5.25) in the following way. Instead of avoiding the poles at  $k' = \pm k$  by following the path  $P_4$  as indicated on Fig. 5.2d, we may keep our integration path along the real axis but displace the poles slightly as pictured in Fig. 5.3. The poles are then at

$$k' = \pm (k + i\varepsilon'), \quad \varepsilon' \rightarrow 0^+, \quad (5.28)$$

where the symbol  $0^+$  means that  $\varepsilon'$  tends to zero while remaining positive. To first order in  $\varepsilon'$ , we then have

$$k'^2 = k^2 + i\varepsilon, \quad \varepsilon \rightarrow 0^+ \quad (5.29)$$



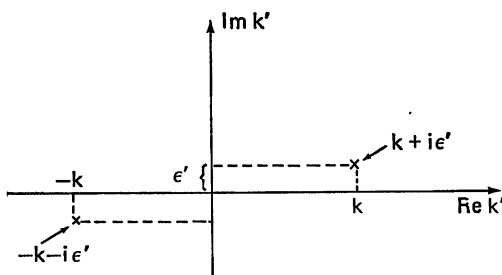


Fig. 5.3. Displacement of the poles in the  $k'$ -plane. The pole at  $k' = k$ , after receiving a small positive imaginary part  $\epsilon'$  has moved slightly off the real axis in the first quadrant of the  $k'$  plane to the position  $k + i\epsilon'$ . The pole at  $k' = -k$  has received an imaginary part  $(-\epsilon')$  and has moved to the position  $-k - i\epsilon'$  in the third quadrant.

where  $\epsilon = 2k\epsilon'$ . Therefore, we obtain the integral representation of  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  in wave vector space as

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') = -(2\pi)^{-3} \lim_{\epsilon \rightarrow 0^+} \int \frac{\exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\}}{k'^2 - k^2 - i\epsilon} d\mathbf{k}'. \quad (5.30)$$

We note that if we define the *Green's function in wave vector space*  $\tilde{G}_0^{(+)}(\mathbf{k}_1, \mathbf{k}_2)$  by the relation

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') = (2\pi)^{-3} \int \exp(-i\mathbf{k}_2 \cdot \mathbf{r}') \tilde{G}_0^{(+)}(\mathbf{k}_1, \mathbf{k}_2) \exp(i\mathbf{k}_1 \cdot \mathbf{r}) d\mathbf{k}_1 d\mathbf{k}_2 \quad (5.31)$$

we find from eq. (5.30) that

$$\tilde{G}_0^{(+)}(\mathbf{k}_1, \mathbf{k}_2) = \lim_{\epsilon \rightarrow 0^+} \frac{\delta(\mathbf{k}_1 - \mathbf{k}_2)}{k^2 - k_1^2 + i\epsilon}. \quad (5.32)$$

### 5.3. The Lippmann-Schwinger equation

We now return to the integral equation (5.9), which we write as

$$\psi_{\mathbf{k}_1}^{(+)}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_1 \cdot \mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k}_1}^{(+)}(\mathbf{r}') d\mathbf{r}' \quad (5.33)$$

where  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  is given by eq. (5.27). This is the integral equation or *Lippmann-Schwinger* [1] *equation* of potential scattering. It replaces the Schrödinger equation (3.19) *plus* the boundary condition (3.27) which is incorporated in eq. (5.33) through the Green's function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$ .

Let us verify that the solution of the Lippmann-Schwinger equation (5.33) has the correct asymptotic behaviour (3.27). The first term on the right of eq. (5.33) has already the required form, so that we only need to analyze the large- $r$  behaviour of the integral

$$J = \int \frac{\exp\{i\mathbf{k}|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}') \psi_{\mathbf{k}_1}^{(+)}(\mathbf{r}') d\mathbf{r}'. \quad (5.34)$$

Since

$$|\mathbf{r} - \mathbf{r}'| = \sqrt{r^2 - 2\mathbf{r} \cdot \mathbf{r}' + r'^2} \xrightarrow{r \rightarrow \infty} r - \hat{\mathbf{p}} \cdot \mathbf{r}' + \frac{1}{2r}(\hat{\mathbf{p}} \times \mathbf{r}')^2 + \cdots \quad (5.35)$$

where  $\hat{\mathbf{p}}$  is the unit vector along  $\mathbf{r}$ , we may write

$$\frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \xrightarrow{r \rightarrow \infty} \frac{\exp(ikr) \exp(-ik\hat{\mathbf{p}} \cdot \mathbf{r}')}{r} \times \left[ 1 + \frac{\hat{\mathbf{p}} \cdot \mathbf{r}'}{r} + \frac{ik}{2r}(\hat{\mathbf{p}} \times \mathbf{r}')^2 + \mathcal{O}(r^{-2}) \right] \quad (5.36)$$

provided that  $r'$  and  $k$  remain finite. Now, for potentials having a finite "range"  $a$  the contribution to the integral (5.34) is negligible when  $r'$  becomes somewhat larger than  $a$ , since  $U(r') \simeq 0$  in that region. Let us set  $r'_{\max} \simeq a$  as a crude estimate of the highest value of  $r'$  to be considered in eq. (5.34). We may then use eq. (5.36) to deduce that for  $r \gg a$  and  $r \gg ka^2$  the integral (5.34) is given by

$$J \simeq \frac{\exp(ikr)}{r} \int \exp(-ik\hat{\mathbf{p}} \cdot \mathbf{r}') U(r') \psi_{k_i}^{(+)}(r') d\mathbf{r}'.$$

Hence, returning to the stationary scattering wave function (5.33) we have

$$\psi_{k_i}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) + \frac{\exp(ikr)}{r} \times \left[ -\frac{1}{4\pi} \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}') U(r') \psi_{k_i}^{(+)}(r') d\mathbf{r}' \right] \quad (5.37)$$

where we have defined the final wave vector

$$\mathbf{k}_f = k\hat{\mathbf{p}}$$

which points in the direction of the detector and has therefore spherical polar coordinates  $(k, \theta, \phi)$ . It is worth noting that our derivation of eq. (5.37) does not apply to the Coulomb potential which has an infinite range.

We now return to the boundary condition (3.27) in which we choose  $A = (2\pi)^{-3/2}$ . Thus we write

$$\psi_{k_i}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) + f(k, \theta, \phi) \frac{\exp(ikr)}{r} \right]. \quad (5.38)$$

Comparing with eq. (5.37), we obtain the *integral representation of the scattering amplitude*

$$f = -\frac{(2\pi)^{3/2}}{4\pi} \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}') U(r') \psi_{k_i}^{(+)}(r') d\mathbf{r}' \quad (5.39)$$

or

$$f = -2\pi^2 \langle \Phi_{k_f} | U | \psi_{k_i}^{(+)} \rangle \quad (5.40)$$

where we have introduced the plane wave  $\Phi_{k_f}$  corresponding to the final wave vector  $k_f$ , namely

$$\Phi_{k_f}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}). \quad (5.41)$$

In terms of the potential  $V(\mathbf{r}) = \hbar^2 U(\mathbf{r})/2m$ , we may also write

$$f = - \frac{(2\pi)^2 m}{\hbar^2} \langle \Phi_{k_f} | V | \psi_{k_i}^{(+)} \rangle. \quad (5.42)$$

The *transition matrix element*  $T_{fi}$  is defined as

$$T_{fi} = \langle \Phi_{k_f} | V | \psi_{k_i}^{(+)} \rangle \quad (5.43)$$

so that

$$f = - \frac{(2\pi)^2 m}{\hbar^2} T_{fi} \quad (5.44)$$

and the differential cross section  $d\sigma/d\Omega = |f|^2$  is given by

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4 m^2}{\hbar^4} |T_{fi}|^2. \quad (5.45)$$

#### 5.4. Compact solutions of the Lippmann–Schwinger equation. Integral representations of the scattering amplitude

Let us return to the Lippmann–Schwinger equation (5.33) and write

$$\psi_{k_i}^{(+)}(\mathbf{r}) = \Phi_{k_i}(\mathbf{r}) + \psi_{sc}^{(+)}(\mathbf{r}) \quad (5.46)$$

where the scattered wave  $\psi_{sc}^{(+)}$  satisfies the inhomogeneous equation

$$[\nabla_{\mathbf{r}}^2 + k^2 - U(\mathbf{r})]\psi_{sc}^{(+)}(\mathbf{r}) = U(\mathbf{r})\Phi_{k_i}(\mathbf{r}). \quad (5.47)$$

Now, suppose that we know the *total* Green's function of the problem  $G^{(+)}(\mathbf{r}, \mathbf{r}')$  satisfying the equation

$$[\nabla_{\mathbf{r}}^2 + k^2 - U(\mathbf{r})]G^{(+)}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (5.48)$$

and such that

$$\psi_{sc}^{(+)}(\mathbf{r}) = \int G^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') d\mathbf{r}' \quad (5.49)$$

corresponds to an outgoing spherical wave. Then we may write explicitly the solution of the Lippmann–Schwinger equation. Using eqs. (5.46) and (5.49), we have

$$\psi_{k_i}^{(+)}(\mathbf{r}) = \Phi_{k_i}(\mathbf{r}) + \int G^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') d\mathbf{r}'. \quad (5.50)$$

In order to determine the total Green's function  $G^{(+)}(\mathbf{r}, \mathbf{r}')$ , let us rewrite eq. (5.48) as

$$[\nabla_{\mathbf{r}}^2 + k^2]G^{(+)}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') + U(\mathbf{r})G^{(+)}(\mathbf{r}, \mathbf{r}'). \quad (5.51)$$

With the help of eq. (5.4) we therefore obtain for  $G^{(+)}(\mathbf{r}, \mathbf{r}')$  the integral equation

$$G^{(+)}(\mathbf{r}, \mathbf{r}') = G_0^{(+)}(\mathbf{r}, \mathbf{r}') + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}'')U(\mathbf{r}'')G^{(+)}(\mathbf{r}'', \mathbf{r}')d\mathbf{r}''. \quad (5.52)$$

The problem of solving the Lippmann–Schwinger equation (5.33) has thus been shifted to that of finding the solution of the integral equation (5.52) for the total Green's function  $G^{(+)}(\mathbf{r}, \mathbf{r}')$ . The relations (5.50) and (5.52) which we have just obtained provide a convenient starting point to discuss various approximation methods. Moreover, we shall see in Part III that relations of this type play an important role in general scattering theory.

We may also use Dirac's bra and ket notation to write the Lippmann–Schwinger equation (5.33) as

$$|\psi_{k_i}^{(+)}\rangle = |\Phi_{k_i}\rangle + G_0^{(+)}U|\psi_{k_i}^{(+)}\rangle \quad (5.53)$$

and the explicit solution (5.50) as

$$|\psi_{k_i}^{(+)}\rangle = |\Phi_{k_i}\rangle + G^{(+)}U|\Phi_{k_i}\rangle \quad (5.54)$$

where the operators  $G^{(+)}$  and  $G_0^{(+)}$  are related by

$$G^{(+)} = G_0^{(+)} + G_0^{(+)}UG^{(+)} \quad (5.55)$$

We note that eqs. (5.53)–(5.55) are written independently of any choice of representation. In the position representation (configuration space) we have

$$\langle \mathbf{r} | \psi_{k_i}^{(+)} \rangle \equiv \psi_{k_i}^{(+)}(\mathbf{r}) \quad (5.56)$$

$$\langle \mathbf{r} | G_0^{(+)} | \mathbf{r}' \rangle \equiv G_0^{(+)}(\mathbf{r}, \mathbf{r}') \quad (5.57)$$

and

$$\langle \mathbf{r} | G^{(+)} | \mathbf{r}' \rangle \equiv G^{(+)}(\mathbf{r}, \mathbf{r}') \quad (5.58)$$

where the Green's functions  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  and  $G^{(+)}(\mathbf{r}, \mathbf{r}')$  are given respectively by eqs. (5.27) and (5.52). Green's operators such as  $G^{(+)}$  and  $G_0^{(+)}$  will be studied in detail in Chapter 14. We also remark that with the help of eq. (5.54) we may rewrite the integral representation (5.40) of the scattering amplitude as

$$f = -2\pi^2 \langle \Phi_{k_i} | U + UG^{(+)}U | \Phi_{k_i} \rangle. \quad (5.59)$$

Let us now consider the Lippmann–Schwinger equation

$$\psi_{k_i}^{(-)}(\mathbf{r}) = (2\pi)^{-3/2} \exp(ik_i \cdot \mathbf{r}) + \int G_0^{(-)}(\mathbf{r}, \mathbf{r}')U(\mathbf{r}')\psi_{k_i}^{(-)}(\mathbf{r}')d\mathbf{r}' \quad (5.60)$$

where

$$G_0^{(-)}(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{\exp\{-ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \quad (5.61)$$

or

$$G_0^{(-)}(\mathbf{r}, \mathbf{r}') = (2\pi)^{-3} \lim_{\varepsilon \rightarrow 0^+} \int \frac{\exp\{ik' \cdot (\mathbf{r} - \mathbf{r}')\}}{k^2 - k'^2 - i\varepsilon} d\mathbf{k}'. \quad (5.62)$$

The wave function  $\psi_{\mathbf{k}_t}^{(-)}(\mathbf{r})$  corresponds to boundary conditions describing an incident plane wave of wave vector  $\mathbf{k}_t$  and an *incoming* spherical wave. Although this wave function does not satisfy the boundary condition (3.27), it nevertheless plays an important role in formal scattering theory, as we shall show in Part III. Introducing also the total Green's function  $G^{(-)}(\mathbf{r}, \mathbf{r}')$  such that

$$G^{(-)}(\mathbf{r}, \mathbf{r}') = G_0^{(-)}(\mathbf{r}, \mathbf{r}') + \int G_0^{(-)}(\mathbf{r}, \mathbf{r}'')U(\mathbf{r}'')G^{(-)}(\mathbf{r}'', \mathbf{r}') d\mathbf{r}'' \quad (5.63)$$

we can write explicitly the solution of eq. (5.60) as

$$\psi_{\mathbf{k}_t}^{(-)}(\mathbf{r}) = \Phi_{\mathbf{k}_t}(\mathbf{r}) + \int G^{(-)}(\mathbf{r}, \mathbf{r}')U(\mathbf{r}')\Phi_{\mathbf{k}_t}(\mathbf{r}')d\mathbf{r}'. \quad (5.64)$$

Using Dirac's notation, we may rewrite the integral equation (5.60) as

$$|\psi_{\mathbf{k}_t}^{(-)}\rangle = |\Phi_{\mathbf{k}_t}\rangle + G_0^{(-)}U|\psi_{\mathbf{k}_t}^{(-)}\rangle \quad (5.65)$$

while the compact solution (5.64) reads

$$|\psi_{\mathbf{k}_t}^{(-)}\rangle = |\Phi_{\mathbf{k}_t}\rangle + G^{(-)}U|\Phi_{\mathbf{k}_t}\rangle. \quad (5.66)$$

Furthermore, we have

$$\langle \mathbf{r}|G_0^{(-)}|\mathbf{r}'\rangle \equiv G_0^{(-)}(\mathbf{r}, \mathbf{r}'), \quad (5.67)$$

$$\langle \mathbf{r}|G^{(-)}|\mathbf{r}'\rangle \equiv G^{(-)}(\mathbf{r}, \mathbf{r}') \quad (5.68)$$

and

$$G^{(-)} = G_0^{(-)} + G_0^{(-)}UG^{(-)}. \quad (5.69)$$

We note from eqs. (5.27) and (5.61) that

$$G_0^{(-)}(\mathbf{r}, \mathbf{r}') = G_0^{(+)*}(\mathbf{r}, \mathbf{r}'). \quad (5.70)$$

Thus, using eqs. (5.52) and (5.63), we deduce that

$$G^{(-)}(\mathbf{r}, \mathbf{r}') = G^{(+)*}(\mathbf{r}, \mathbf{r}') \quad (5.71)$$

and therefore

$$G^{(-)} = G^{(+)\dagger} \quad (5.72)$$

where the dagger denotes hermitian conjugation. Hence, from eqs. (5.66) and (5.72) we obtain

$$\langle \psi_{\mathbf{k}_t}^{(-)}| = \langle \Phi_{\mathbf{k}_t}| + \langle \Phi_{\mathbf{k}_t}|UG^{(+)} \quad (5.73)$$

so that, by comparison with eq. (5.59), we deduce another important integral representation of the scattering amplitude, namely

$$f = -2\pi^2 \langle \psi_{\mathbf{k}_t}^{(-)}|U|\Phi_{\mathbf{k}_t}\rangle. \quad (5.74)$$

### 5.5. Partial wave analysis of the Lippmann–Schwinger equation

In this section we shall consider the particular case of a central potential  $V(r)$ . Following the ideas of Section 4.1 it is then natural to substitute the

expansion (4.62b) in the Lippmann–Schwinger equation (5.33), namely

$$\psi_{\mathbf{k}_i}^{(+)}(k, \mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_l R_l(k, r) Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{lm}(\hat{\mathbf{r}}) \quad (5.75)$$

where the coefficients  $c_l$  depend on the “normalization” adopted for the radial functions  $R_l$  and we have also used eq. (4.30).

Since we have [see eq. (4.31)]

$$\exp(i\mathbf{k} \cdot \mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{lm}(\hat{\mathbf{r}}) \quad (5.76)$$

the corresponding development of the incident plane wave is simply

$$\Phi_{\mathbf{k}_i}(\mathbf{r}) = (2/\pi)^{1/2} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{lm}(\hat{\mathbf{r}}). \quad (5.77)$$

We also need the expansion of  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  in spherical harmonics. Because  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  only depends on  $|\mathbf{r} - \mathbf{r}'|$ , i.e. on  $r, r'$  and on the angle  $\theta_0$  between the vectors  $\mathbf{r}$  and  $\mathbf{r}'$ , we may write

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} g_l^{(+)}(r, r') Y_{lm}^*(\hat{\mathbf{r}}) Y_{lm}(\hat{\mathbf{r}}'). \quad (5.78)$$

The functions  $g_l^{(+)}(r, r')$  may be determined by using the integral representation of  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  in momentum space, given by eq. (5.30). Expanding the plane waves  $\exp(i\mathbf{k}' \cdot \mathbf{r})$  and  $\exp(-i\mathbf{k}' \cdot \mathbf{r}')$  in spherical harmonics according to eq. (5.76), we find that

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') = -\frac{2}{\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}^*(\hat{\mathbf{r}}) Y_{lm}(\hat{\mathbf{r}}') \int_0^{\infty} dk' k'^2 \frac{j_l(k'r) j_l(k'r')}{k'^2 - k^2 - i\varepsilon} \quad (5.79)$$

and therefore

$$g_l^{(+)}(r, r') = -\frac{2}{\pi} \int_0^{\infty} dk' k'^2 \frac{j_l(k'r) j_l(k'r')}{k'^2 - k^2 - i\varepsilon}. \quad (5.80)$$

Moreover, since  $j_l(-z) = (-)^l j_l(z)$  (see Appendix C) we may also write eq. (5.80) as

$$g_l^{(+)}(r, r') = -\frac{1}{\pi} \int_{-\infty}^{+\infty} dk' k'^2 \frac{j_l(k'r) j_l(k'r')}{k'^2 - k^2 - i\varepsilon}. \quad (5.81)$$

This expression is readily evaluated by contour integration in the complex  $k'$ -plane. Because  $j_l(z)$  is an entire function of  $z$  (i.e. is an analytic function of  $z$  in the open  $z$ -plane) the only singularities of the integrand are the two poles of the denominator. Moreover, in order to apply a method similar to the one we used in Section 5.2, we note that (see Appendix C)

$$j_l = \frac{1}{2}[h_l^{(1)} + h_l^{(2)}] \quad (5.82)$$

while

$$h_l^{(1)}(z) \xrightarrow{|z| \rightarrow \infty} -i \frac{\exp\{i(z - \frac{1}{2}l\pi)\}}{z} \quad (5.83a)$$

and

$$h_l^{(2)}(z) \xrightarrow{|z| \rightarrow \infty} i \frac{\exp\{-i(z - \frac{1}{2}l\pi)\}}{z}. \quad (5.83b)$$

Consider first the case  $r < r'$ . Using eq. (5.82) to write  $j_l(k'r') = \frac{1}{2}[h_l^{(1)}(k'r') + h_l^{(2)}(k'r')]$  and substituting in eq. (5.81) we break the integral in two parts as

$$g_l^{(+)}(r, r') = J_1 + J_2 \quad (5.84)$$

where

$$J_1 = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} dk' k'^2 \frac{j_l(k'r) h_l^{(1)}(k'r')}{k'^2 - k^2 - i\epsilon} \quad (5.85)$$

and

$$J_2 = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} dk' k'^2 \frac{j_l(k'r) h_l^{(2)}(k'r')}{k'^2 - k^2 - i\epsilon}. \quad (5.86)$$

Now, from eqs. (5.82) and (5.83) we see that for  $r < r'$  and as  $|k'| \rightarrow \infty$ , the quantity  $j_l(k'r) h_l^{(1)}(k'r')$  decreases exponentially in the *upper* half  $k'$ -plane ( $\text{Im } k' > 0$ ), while  $j_l(k'r) h_l^{(2)}(k'r')$  decreases exponentially in the *lower* half  $k'$ -plane ( $\text{Im } k' < 0$ ). We may thus close the contour of  $J_1$  by a large semi-circle in the upper half-plane, while we add a large semi-circle in the lower half-plane to the integration path of  $J_2$ . Applying Cauchy's theorem and remembering that  $j_l(-z) = (-)^l j_l(z)$  and  $h_l^{(2)}(-z) = (-)^l h_l^{(1)}(z)$  we obtain for  $r < r'$

$$g_l^{(+)}(r, r') = -ik j_l(kr) h_l^{(1)}(kr'). \quad (5.87a)$$

When  $r > r'$  a similar reasoning leads to the result

$$g_l^{(+)}(r, r') = -ik j_l(kr') h_l^{(1)}(kr). \quad (5.87b)$$

We may therefore summarize eqs. (5.87) by writing

$$g_l^{(+)}(r, r') = -ik j_l(kr_{<}) h_l^{(1)}(kr_{>}) \quad (5.88)$$

where  $r_{<}$  is the lesser and  $r_{>}$  the greater of  $r$  and  $r'$ . Hence, returning to eq. (5.78) we have

$$G_0^{(+)}(r, r') = -ik \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} j_l(kr_{<}) h_l^{(1)}(kr_{>}) Y_{lm}^*(\hat{r}') Y_{lm}(\hat{r}). \quad (5.89)$$

With the expansions (5.75), (5.77) and (5.89) at our disposal we are now ready to carry out the partial wave analysis of the Lippmann-Schwinger equation. Substituting in eq. (5.33) and using the orthonormality property of the spherical harmonics we find that

$$\begin{aligned} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_l R_l(k, r) Y_{lm}^*(\hat{k}_i) Y_{lm}(\hat{r}) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \left\{ (2/\pi)^{1/2} i^l j_l(kr) \right. \\ &\quad \left. - ik c_l \int_0^{\infty} j_l(kr_{<}) h_l^{(1)}(kr_{>}) U(r') R_l(k, r') r'^2 dr' \right\} Y_{lm}^*(\hat{k}_i) Y_{lm}(\hat{r}) \end{aligned} \quad (5.90)$$

so that

$$c_l R_l(k, r) = (2/\pi)^{1/2} i^l j_l(kr) - ikc_l \int_0^\infty j_l(kr_<) h_l^{(1)}(kr_>) U(r') R_l(k, r') r'^2 dr'. \quad (5.91)$$

We may also write more explicitly

$$\begin{aligned} c_l R_l(k, r) = (2/\pi)^{1/2} i^l j_l(kr) - ikc_l h_l^{(1)}(kr) \int_0^r j_l(kr') U(r') R_l(k, r') r'^2 dr' \\ - ikc_l j_l(kr) \int_r^\infty h_l^{(1)}(kr') U(r') R_l(k, r') r'^2 dr'. \end{aligned} \quad (5.92)$$

Let us now examine the asymptotic behaviour of this equation when  $r \rightarrow \infty$ . In this case the last term vanishes and we have

$$\begin{aligned} R_l(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) \left[ (2/\pi)^{1/2} \frac{i^l}{c_l} - ik \int_0^\infty j_l(kr') U(r') R_l(k, r') r'^2 dr' \right] \\ + n_l(kr) \left[ k \int_0^\infty j_l(kr') U(r') R_l(k, r') r'^2 dr' \right] \end{aligned} \quad (5.93)$$

where we have used the fact that  $h_l^{(1)} = j_l + in_l$ . Upon comparison with eq. (4.86b) we immediately deduce that

$$\tan \delta_l = \frac{-k \int_0^\infty j_l(kr) U(r) R_l(k, r) r^2 dr}{(2/\pi)^{1/2} (i^l/c_l) - ik \int_0^\infty j_l(kr) U(r) R_l(k, r) r^2 dr}. \quad (5.94)$$

So far we have left the coefficients  $c_l$  unspecified. An obvious choice consists in requiring that

$$c_l = \frac{(2/\pi)^{1/2} i^l}{1 + ik \int_0^\infty j_l(kr) U(r) R_l(k, r) r^2 dr} \quad (5.95)$$

so that eq. (5.94) reduces to

$$\tan \delta_l = -k \int_0^\infty j_l(kr) U(r) R_l(k, r) r^2 dr \quad (5.96)$$

and eq. (5.93) now reads [compare with eq. (4.86b)]

$$R_l(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) - \tan \delta_l n_l(kr). \quad (5.97)$$

With the "normalization" of our radial functions determined in this way we may now return to eq. (5.92). Using eq. (5.95) and the fact that  $h_l^{(1)} = j_l + in_l$ , we then find that the functions  $R_l(k, r)$  satisfy the integral equations

$$R_l(k, r) = j_l(kr) + \int_0^\infty G_l(r, r') U(r') R_l(k, r') r'^2 dr' \quad (5.98)$$

with

$$G_l(r, r') = -kj_l(kr_<)n_l(kr_>). \quad (5.99)$$



## 5.6. The Lippmann–Schwinger equation and the Fredholm method

We first summarize some mathematical results pertaining to the theory of integral equations [e.g. 4]. Let us start with the integral equation

$$f(x) = g(x) + \lambda \int_a^b K(x, y) f(y) dy \quad (5.100)$$

where  $\lambda$  is a parameter,  $g(x)$  is a continuous function for  $a \leq x \leq b$  and the kernel  $K(x, y)$  is continuous and finite, i.e.

$$|K(x, y)| \leq M = \text{const.} \quad (5.101)$$

in the domain  $a \leq x \leq b$ ;  $a \leq y \leq b$ .

We define the *Fredholm determinant*

$$d(\lambda) = 1 + \sum_{n=1}^{\infty} \frac{(-\lambda)^n}{n!} \int_a^b dx_1 \dots \int_a^b dx_n \begin{vmatrix} K(x_1, x_1) & \dots & K(x_1, x_n) \\ \vdots & & \vdots \\ K(x_n, x_1) & \dots & K(x_n, x_n) \end{vmatrix} \quad (5.102)$$

and the *first Fredholm minor*

$$D(\lambda; x, y) = K(x, y) + \sum_{n=1}^{\infty} \frac{(-\lambda)^n}{n!} \int_a^b dx_1 \dots \int_a^b dx_n \begin{vmatrix} K(x, y) & K(x, x_1) & \dots & K(x, x_n) \\ K(x_1, y) & K(x_1, x_1) & \dots & K(x_1, x_n) \\ \vdots & \vdots & & \vdots \\ K(x_n, y) & K(x_n, x_1) & \dots & K(x_n, x_n) \end{vmatrix}. \quad (5.103)$$

Then, if  $\lambda$  is not a zero of  $d(\lambda)$ , the integral equation (5.100) has a unique continuous solution, namely

$$f(x) = g(x) + \int_a^b \frac{D(\lambda; x, y)}{d(\lambda)} g(y) dy. \quad (5.104)$$

This result may be generalized in several ways; it is valid for:

1) Functions  $g(x)$  which are no longer continuous, but square integrable (denoted as  $g(x) \in \mathcal{L}^2$ ), i.e. such that

$$\int_a^b |g(x)|^2 dx < \infty. \quad (5.105)$$

2) Kernels  $K(x, y)$  which belong to the Hilbert–Schmidt class (denoted by  $K(x, y) \in \mathcal{L}^2$ ). If we define the norm  $\|K\|$  of the kernel by

$$\|K\| = \left[ \int_a^b dx \int_a^b dy |K(x, y)|^2 \right]^{1/2} \quad (5.106)$$

the condition  $K(x, y) \in \mathcal{L}^2$  means that

$$a) \|K\|^2 < \infty. \quad (5.107a)$$

$$b) \text{ For every } x, \int_a^b |K(x, y)|^2 dy < \infty. \quad (5.107b)$$

$$c) \text{ For every } y, \int_a^b |K(x, y)|^2 dx < \infty. \quad (5.107c)$$

If the conditions (b) and (c) are suppressed, the kernel is said to belong to the Hilbert–Schmidt class in the generalized sense.

3) Infinite intervals and an arbitrary number of dimensions.

In these cases the corresponding solution, given by the generalization of eq. (5.104) will now be square integrable.

Let us try to apply these results to the Lippmann–Schwinger equation (5.33). In the following discussion it is convenient to consider the slightly more general equation

$$\psi_{k_1}^{(+)}(\mathbf{r}) = \Phi_{k_1}(\mathbf{r}) + \lambda \int K(\mathbf{r}, \mathbf{r}') \psi_{k_1}^{(+)}(\mathbf{r}') d\mathbf{r}' \quad (5.108)$$

where the kernel  $K(\mathbf{r}, \mathbf{r}')$  is given by

$$K(\mathbf{r}, \mathbf{r}') = -\frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{4\pi|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}') \quad (5.109)$$

and we have introduced the parameter  $\lambda$ .

To investigate if the kernel (5.109) belongs to the Hilbert–Schmidt class (in the generalized sense), it is convenient to let  $k$  become complex, so that

$$k = \text{Re } k + i \text{Im } k. \quad (5.110)$$

Then the condition (5.107a) yields

$$\int d\mathbf{r} \int d\mathbf{r}' |K(\mathbf{r}, \mathbf{r}')|^2 = \frac{1}{16\pi^2} \int d\mathbf{r} d\mathbf{r}' \frac{\exp\{-2|\mathbf{r} - \mathbf{r}'| \text{Im } k\}}{|\mathbf{r} - \mathbf{r}'|^2} |U(\mathbf{r}')|^2 < \infty. \quad (5.111)$$

Let us change variables from  $\mathbf{r}$  to  $\mathbf{s}$  defined by

$$\mathbf{s} = \mathbf{r} - \mathbf{r}' \quad (5.112)$$

so that the Jacobian of the transformation is unity. Hence (5.111) reads

$$\frac{1}{16\pi^2} \int d\mathbf{r}' |U(\mathbf{r}')|^2 \int d\mathbf{s} \frac{\exp\{-2s \text{Im } k\}}{s^2} < \infty \quad (5.113)$$

from which we conclude that if

$$i) \text{Im } k > 0 \quad (5.114)$$

and

$$ii) \int d\mathbf{r}' |U(\mathbf{r}')|^2 < \infty \quad (5.115)$$

the Fredholm theory can be applied to eq. (5.108). Since

$$E = \hbar^2 k^2 / 2m \quad (5.116)$$

we may also transpose our discussion to the complex energy plane. For this purpose, it is convenient to imagine the complex  $E$  plane as formed of two superposed *Riemann sheets* corresponding to the two possible choices:  $\text{Im } k > 0$  or  $\text{Im } k < 0$ . For each choice, we see that the relation (5.116) transforms one half- $k$ -plane onto an entire sheet of the complex  $E$  plane. We define the Riemann sheet corresponding to the choice  $\text{Im } k > 0$  as the “*physical*” sheet, while the sheet which corresponds to  $\text{Im } k < 0$  is denoted as the “*unphysical*” sheet [5]. These two sheets have the common boundary  $\text{Im } k = 0$ , so that it is convenient to consider the complex  $E$  plane as cut along the real axis from 0 to  $\infty$  (see Fig. 5.4).

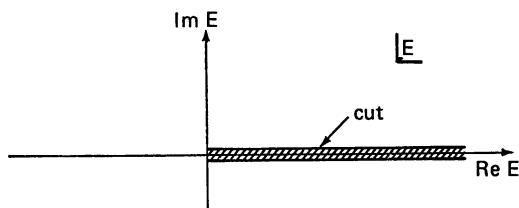


Fig. 5.4. The complex energy plane. The cut which runs along the real axis from  $E = 0$  to  $E = +\infty$  is the common boundary of the “physical” and “unphysical” sheets corresponding respectively to  $\text{Im } k > 0$  and  $\text{Im } k < 0$ .

As  $k$  becomes real, i.e. when  $E$  approaches the cut, we see from eq. (5.113) that the kernel  $K(\mathbf{r}, \mathbf{r}')$  of the Lippmann–Schwinger equation is no longer in the Hilbert–Schmidt class. Hence the Fredholm theory cannot be applied directly to the Lippmann–Schwinger equation for *real* values of  $k$ , i.e. for  $E$  real and positive. Since we are precisely interested in real values of  $k$  and  $E$  such that  $k \geq 0$  and  $E \geq 0$ , we meet here a genuine difficulty.

However, there are several ways to overcome this problem [e.g. 6, 7]. The first one is to write

$$U(\mathbf{r}) = |U(\mathbf{r})|\eta(\mathbf{r}) \quad (5.117)$$

where

$$\eta(\mathbf{r}) = \begin{cases} +1 & \text{if } U(\mathbf{r}) > 0 \\ -1 & \text{if } U(\mathbf{r}) < 0 \end{cases} \quad (5.118)$$

and to multiply the Lippmann–Schwinger equation (5.108) by  $|U|^{1/2}$ .

Defining the quantities

$$\tilde{\psi}_{k_1}^{(+)}(\mathbf{r}) = |U|^{1/2}\psi_{k_1}^{(+)}(\mathbf{r}) \quad (5.119)$$

$$\tilde{\Phi}_{k_1}(\mathbf{r}) = |U|^{1/2}\Phi_{k_1}(\mathbf{r}) \quad (5.120)$$

and

$$\tilde{K}(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi}|U(\mathbf{r})|^{1/2}\frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|}|U(\mathbf{r}')|^{1/2}\eta(\mathbf{r}'), \quad (5.121)$$

we obtain the new integral equation

$$\tilde{\psi}_{k_1}^{(+)}(\mathbf{r}) = \tilde{\Phi}_{k_1}(\mathbf{r}) + \lambda \int \tilde{K}(\mathbf{r}, \mathbf{r}') \tilde{\psi}_{k_1}^{(+)}(\mathbf{r}') d\mathbf{r}'. \quad (5.122)$$

Let us examine the kernel  $\tilde{K}(\mathbf{r}, \mathbf{r}')$ . We now have

$$\int d\mathbf{r} d\mathbf{r}' |\tilde{K}(\mathbf{r}, \mathbf{r}')|^2 = \frac{1}{16\pi^2} \int d\mathbf{r} d\mathbf{r}' |U(\mathbf{r})| |U(\mathbf{r}')| \frac{\exp\{-2|\mathbf{r} - \mathbf{r}'| \operatorname{Im} k\}}{|\mathbf{r} - \mathbf{r}'|^2} \quad (5.123)$$

so that

$$\int d\mathbf{r} d\mathbf{r}' |\tilde{K}(\mathbf{r}, \mathbf{r}')|^2 \leq \frac{1}{16\pi^2} \int d\mathbf{r} d\mathbf{r}' |U(\mathbf{r})| |U(\mathbf{r}')| \frac{1}{|\mathbf{r} - \mathbf{r}'|^2}. \quad (5.124)$$

Thus, the quantity on the right-hand side of eq. (5.123) is finite, even for  $\operatorname{Im} k = 0$  if

$$\text{i) } \int d\mathbf{r} |U(\mathbf{r})| < \infty \quad (5.125)$$

and

$$\text{ii) } \int d\mathbf{r}' |U(\mathbf{r}')| / |\mathbf{r} - \mathbf{r}'|^2 \leq M < \infty \quad (5.126)$$

where  $M$  is some positive constant.

The inequalities (5.125) and (5.126) provide *sufficient conditions* for the applicability of the Fredholm theory to the modified Lippmann-Schwinger equation (5.122).

Another way of making the Fredholm theory applicable to the Lippmann-Schwinger equation (5.108) is to first iterate [8, 9] this equation. This leads to the integral equation

$$\psi_{k_1}^{(+)}(\mathbf{r}) = F_{k_1}(\mathbf{r}) + \lambda^2 \int K_2(\mathbf{r}, \mathbf{r}') \psi_{k_1}^{(+)}(\mathbf{r}') d\mathbf{r}' \quad (5.127)$$

where

$$F_{k_1}(\mathbf{r}) = \Phi_{k_1}(\mathbf{r}) + \lambda \int K(\mathbf{r}, \mathbf{r}') \Phi_{k_1}(\mathbf{r}') d\mathbf{r}' \quad (5.128)$$

and

$$K_2(\mathbf{r}, \mathbf{r}') = \int K(\mathbf{r}, \mathbf{r}'') K(\mathbf{r}'', \mathbf{r}') d\mathbf{r}''. \quad (5.129)$$

Let us write the iterated kernel  $K_2(\mathbf{r}, \mathbf{r}')$  explicitly as

$$\begin{aligned} K_2(\mathbf{r}, \mathbf{r}') &= \frac{1}{16\pi^2} \int d\mathbf{r}'' \frac{\exp\{ik[|\mathbf{r} - \mathbf{r}''| + |\mathbf{r}'' - \mathbf{r}'|]\}}{|\mathbf{r} - \mathbf{r}''| |\mathbf{r}'' - \mathbf{r}'|} U(\mathbf{r}'') U(\mathbf{r}') \\ &= \frac{1}{16\pi^2} U(\mathbf{r}') \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{r'} A(\mathbf{r}, \mathbf{r}') \end{aligned} \quad (5.130)$$

where

$$A(\mathbf{r}, \mathbf{r}') = r' \int d\mathbf{r}'' U(\mathbf{r}'') \frac{\exp\{ik[|\mathbf{r} - \mathbf{r}''| + |\mathbf{r}'' - \mathbf{r}'| - |\mathbf{r} - \mathbf{r}'|]\}}{|\mathbf{r} - \mathbf{r}''| |\mathbf{r}'' - \mathbf{r}'|}. \quad (5.131)$$

From the triangular inequality

$$|\mathbf{r} - \mathbf{r}''| + |\mathbf{r}'' - \mathbf{r}'| \geq |\mathbf{r} - \mathbf{r}'| \quad (5.132)$$

we deduce that, for all  $\text{Im } k \geq 0$

$$|A(\mathbf{r}, \mathbf{r}')| \leq r' \int d\mathbf{r}'' \frac{|U(\mathbf{r}'')|}{|\mathbf{r} - \mathbf{r}''| |\mathbf{r}'' - \mathbf{r}'|} = B(\mathbf{r}, \mathbf{r}'). \quad (5.133)$$

In the particular case of a central potential such that

$$\int_0^\infty dr r |U(r)| < \infty \quad (5.134)$$

and

$$r^2 |U(r)| \leq M < \infty. \quad (5.135)$$

Jost and Pais [8] have shown that  $B(\mathbf{r}, \mathbf{r}') \leq N < \infty$ . Here  $M$  and  $N$  are positive constants. Then, from eq. (5.133)

$$|A(\mathbf{r}, \mathbf{r}')| \leq N < \infty \quad (5.136)$$

and the Fredholm theory can be applied to eq. (5.127). The solution can then be written as

$$\psi_{k_1}^{(+)}(\mathbf{r}) = F_{k_1}(\mathbf{r}) + \int \frac{D_2(\lambda^2; \mathbf{r}, \mathbf{r}')}{d_2(\lambda^2)} F_{k_1}(\mathbf{r}') d\mathbf{r}' \quad (5.137)$$

with the Fredholm determinant

$$d_2(\lambda^2) = 1 + \sum_{n=1}^{\infty} \frac{(-\lambda^2)^n}{n!} \int d\mathbf{r}_1 \dots \int d\mathbf{r}_n \begin{vmatrix} K_2(\mathbf{r}_1, \mathbf{r}_1) & \dots & K_2(\mathbf{r}_1, \mathbf{r}_n) \\ \vdots & & \vdots \\ K_2(\mathbf{r}_n, \mathbf{r}_1) & \dots & K_2(\mathbf{r}_n, \mathbf{r}_n) \end{vmatrix} \quad (5.138)$$

and the first Fredholm minor

$$D_2(\lambda^2; \mathbf{r}, \mathbf{r}') = K_2(\mathbf{r}, \mathbf{r}') + \sum_{n=1}^{\infty} \frac{(-\lambda^2)^n}{n!} \int d\mathbf{r}_1 \dots \int d\mathbf{r}_n \begin{vmatrix} K_2(\mathbf{r}, \mathbf{r}') & K_2(\mathbf{r}, \mathbf{r}_1) & \dots & K_2(\mathbf{r}, \mathbf{r}_n) \\ K_2(\mathbf{r}_1, \mathbf{r}') & K_2(\mathbf{r}_1, \mathbf{r}_1) & \dots & K_2(\mathbf{r}_1, \mathbf{r}_n) \\ \vdots & & & \vdots \\ K_2(\mathbf{r}_n, \mathbf{r}') & K_2(\mathbf{r}_n, \mathbf{r}_1) & \dots & K_2(\mathbf{r}_n, \mathbf{r}_n) \end{vmatrix}. \quad (5.139)$$

The representation (5.137)–(5.139) of the solution has the disadvantage that the quantity  $d_2(\lambda^2)$  vanishes for  $\lambda = \pm \lambda_n$ , where  $\lambda_n$  are the eigenvalues of the original integral equation. One can therefore factor out an entire function in  $D_2(\lambda^2; \mathbf{r}, \mathbf{r}')$  and  $d_2(\lambda^2)$ , as was first demonstrated by Poincaré [10].

To summarize, the Fredholm theory can be applied to a slightly modified version of the Lippmann–Schwinger equation. The series (5.102)–(5.103) or (5.138)–(5.139) converge uniformly and absolutely. Moreover, as Jost and Pais have shown [8], the scattering wave function  $\psi_{k_i}^{(+)}(\mathbf{r})$  has no singularity for real values of  $k$ , except perhaps at  $k = 0$ . It should be noted, however, that the convergence of the Fredholm series is often slow, which makes the use of the method a rather tedious affair. If the equation can be reduced to one dimensional equations as in Section 5.5 [see eq. (5.98)] then appropriate matrix inversion techniques can be used in the numerical solution of the problem.

### 5.7. Non-local potentials

We conclude this chapter by an extension of the Lippmann–Schwinger equation to the case of scattering by non-local interactions.

A non-local potential is an operator which plays the role of the potential in the Schrödinger equation but is not diagonal in the coordinate representation [11]. In other words, its matrix elements in that representation read

$$\langle \mathbf{r} | V | \mathbf{r}' \rangle. \quad (5.140)$$

The action of a non-local potential on a wave function  $\psi(\mathbf{r})$  is therefore described by the integral operator

$$\int \langle \mathbf{r} | V | \mathbf{r}' \rangle \psi(\mathbf{r}') d\mathbf{r}'. \quad (5.141)$$

Thus the action of the non-local potential on the wave function depends on the value of this function in all configuration space. This non-locality property justifies the name of the potential. By contrast, one has for a local potential

$$\langle \mathbf{r} | V | \mathbf{r}' \rangle = V(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') \quad (5.142)$$

so that in that case

$$\int \langle \mathbf{r} | V | \mathbf{r}' \rangle \psi(\mathbf{r}') d\mathbf{r}' = V(\mathbf{r})\psi(\mathbf{r}). \quad (5.143)$$

The Schrödinger equation for a non-local interaction now becomes an integro-differential equation, namely

$$[\nabla_{\mathbf{r}}^2 + k^2]\psi(\mathbf{r}) = \int \langle \mathbf{r} | U | \mathbf{r}' \rangle \psi(\mathbf{r}') d\mathbf{r}' \quad (5.144)$$

where we have defined

$$\langle \mathbf{r} | U | \mathbf{r}' \rangle = \frac{2m}{\hbar^2} \langle \mathbf{r} | V | \mathbf{r}' \rangle. \quad (5.145)$$

A straightforward generalization of the arguments of Section 5.1 then leads to the Lippmann–Schwinger equation for non-local interactions, namely

$$\psi_{k_i}^{(+)}(\mathbf{r}) = \Phi_{k_i}(\mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') \langle \mathbf{r}' | U | \mathbf{r}'' \rangle \psi_{k_i}^{(+)}(\mathbf{r}'') d\mathbf{r}' d\mathbf{r}'' \quad (5.146)$$

where  $\Phi_{\mathbf{k}_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r})$  and the Green's function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  is given by eq. (5.27). The integral representation of the scattering amplitude is still [see eq. (5.40)]

$$f = -2\pi^2 \langle \Phi_{\mathbf{k}_i} | U | \psi_{\mathbf{k}_i}^{(+)} \rangle \quad (5.147)$$

or explicitly

$$f = -2\pi^2 \int \Phi_{\mathbf{k}_i}^*(\mathbf{r}) \langle \mathbf{r} | U | \mathbf{r}' \rangle \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (5.148)$$

where  $\Phi_{\mathbf{k}_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r})$ .

As an example, let us consider the *separable* [12] non-local interaction

$$\langle \mathbf{r} | U | \mathbf{r}' \rangle = \lambda u(\mathbf{r}) u(\mathbf{r}'), \quad (5.149)$$

where we assume that  $u(\mathbf{r})$  is a real function. With such a potential, the scattering amplitude (5.148) becomes

$$f = -2\pi^2 \lambda \langle \Phi_{\mathbf{k}_i} | u \rangle \langle u | \psi_{\mathbf{k}_i}^{(+)} \rangle. \quad (5.150)$$

However, from eq. (5.146) we obtain

$$\langle u | \psi_{\mathbf{k}_i}^{(+)} \rangle = \langle u | \Phi_{\mathbf{k}_i} \rangle + \lambda \langle u | G_0^{(+)} | u \rangle \langle u | \psi_{\mathbf{k}_i}^{(+)} \rangle \quad (5.151)$$

with

$$\langle u | G_0^{(+)} | u \rangle = \int u(\mathbf{r}) G_0^{(+)}(\mathbf{r}, \mathbf{r}') u(\mathbf{r}') d\mathbf{r} d\mathbf{r}'. \quad (5.152)$$

Hence

$$\langle u | \psi_{\mathbf{k}_i}^{(+)} \rangle = \frac{\langle u | \Phi_{\mathbf{k}_i} \rangle}{1 - \lambda \langle u | G_0^{(+)} | u \rangle}. \quad (5.153)$$

Substituting this result in eq. (5.150), we find that

$$f = -2\pi^2 \lambda \frac{\langle \Phi_{\mathbf{k}_i} | u \rangle \langle u | \Phi_{\mathbf{k}_i} \rangle}{1 - \lambda \langle u | G_0^{(+)} | u \rangle}. \quad (5.154)$$

For simple choices of the function  $u(\mathbf{r})$ , this expression can be evaluated in closed form to give an exact, explicit expression of the scattering amplitude. We shall illustrate the use of eq. (5.154) at the end of Chapter 8 in connection with our study of the Born series.

## References and notes

- [1] LIPPMANN, B. A. and J. SCHWINGER (1950), Phys. Rev. **79**, 469.
- [2] For a general discussion of Green's functions, see for example  
 COURANT, R. and D. HILBERT (1966), *Methods of Mathematical Physics* (Interscience Publ., New York) Vol. I, Chapter 5; Vol. II, Chapter 4;  
 MORSE, P. M. and H. FESHBAH (1953), *Methods of Theoretical Physics* (McGraw-Hill, New York) Chapter 7;  
 BYRON Jr., F. W. and R. W. FULLER (1970), *Mathematics of Classical and Quantum Physics* (Addison-Wesley, Reading, Mass.) Chapter 7.

- [3] In order to simplify the notation, we still omit to indicate explicitly the  $k$ -dependence of the functions  $G_0, g_0$ , etc.
- [4] RIESZ, F. and B. SZ. NAGY (1955), *Functional Analysis* (F. Ungar Publ. Co., New York) Chapter 4;  
     COURANT, R. and D. HILBERT, loc. cit. [2] Vol. I, Chapter 3;  
     SMITHIES, F. (1958), *Integral Equations* (Cambridge Univ. Press, New York);  
     BYRON JR., F. W. and R. W. FULLER, loc. cit. [2] Chapters 8 and 9.
- [5] One should not attach too much importance to the terms "physical" and "unphysical". Both sheets are used in the interpretation of physical phenomena, as we shall see later. Strictly speaking, of course, "physics" lies on the real axis of the  $E$ -plane.
- [6] SMITHIES, F., loc. cit. [4].
- [7] NEWTON, R. (1966), *Scattering Theory of Waves and Particles* (McGraw-Hill, New York) Chapters 9, 10.
- [8] JOST, R. and A. PAIS (1951), Phys. Rev. **82**, 840.
- [9] KHURI, N. N. (1957), Phys. Rev. **107**, 1148.
- [10] POINCARÉ, H. (1901), Acta Math. **33**, 57.
- [11] The Green's functions introduced above provide other examples of non-local operators in the coordinate representation.
- [12] Apart from its interest in potential scattering, the separable potential has played an important role in recent studies of the three-body problem. We shall return to this point in Chapter 19.



## The Coulomb Potential

The Coulomb interaction potential for two particles having respectively the electric charges  $Z_1e$  and  $Z_2e$  is

$$V_c(r) = Z_1Z_2e^2/r. \quad (6.1)$$

Many results which have been derived in the previous chapters are not directly applicable to this potential. The physical reason for such an exceptional behaviour is that the Coulomb potential has an infinite “range” (corresponding to the zero mass of the photon), so that its influence is felt even for  $r \rightarrow \infty$ . In other words, all incoming particles – even those corresponding to very large impact parameters – are scattered by the Coulomb potential. Hence, the Coulomb scattering wave functions do not satisfy the boundary condition (3.27).

Of course, in actual physical situations the Coulomb field (6.1) is shielded by other charges so that the “pure” Coulomb expression (6.1) is replaced by a “screened” Coulomb potential

$$V(r) = V_c(r)s(r) \quad (6.2)$$

where  $s(r)$  is a screening function. For example, in most nuclear and high-energy scattering processes one may assume that  $s(r) = 0$  for  $r > R_s$ , where  $R_s$  is the screening distance at which the two charges are shielded from each other. Indeed, the relevant collision distances in those processes are of the order of  $10^{-13}$  cm, while the screening distance  $R_s$ , due to the presence of the atomic electrons, is about  $10^{-8}$  cm. A convenient expression of the screening function, which is often used in these cases, is given by the simple form

$$s(r) = \begin{cases} 1 & \text{for } r < R_s \\ 0 & \text{for } r > R_s. \end{cases} \quad (6.3)$$

Despite the fact that a pure Coulomb field is an idealization, the solution of the scattering problem for such a potential is of great importance, particularly in atomic and nuclear physics. We shall outline here two ways of treating the Coulomb potential. The first and simpler one uses *parabolic coordinates*, and is described in Section 6.1. In Section 6.2 we shall return to *spherical polar coordinates* and make the necessary modifications to the method of partial waves. Finally, we study in Section 6.3 the situation where a short range potential is added to the Coulomb field. More details about the treatment of the Coulomb potential in scattering theory may be found in the references [1] to [5] listed at the end of this chapter.

### 6.1. The Coulomb potential in parabolic coordinates

Let us define the parabolic coordinates  $(\xi, \eta, \phi)$  through the relations

$$\begin{aligned} x &= \sqrt{\xi\eta} \cos \phi, \\ y &= \sqrt{\xi\eta} \sin \phi, \\ z &= \frac{1}{2}(\xi - \eta), \\ \xi &= r + z = r(1 + \cos \phi), \\ \eta &= r - z = r(1 - \cos \phi), \\ \phi &= \tan^{-1}(y/x). \end{aligned} \quad (6.4)$$

The surfaces  $\xi = \text{const.}$  and  $\eta = \text{const.}$  are paraboloids of revolution about the  $z$  axis with the origin as focus.

The operator  $\nabla^2$  is given in these coordinates by

$$\nabla^2 = \frac{4}{\xi + \eta} \left[ \frac{\partial}{\partial \xi} \left( \xi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \eta \frac{\partial}{\partial \eta} \right) \right] + \frac{1}{\xi\eta} \frac{\partial^2}{\partial \phi^2} \quad (6.5)$$

so that the Schrödinger equation corresponding to the pure Coulomb potential (6.1) becomes

$$-\frac{\hbar^2}{2m} \left\{ \frac{4}{\xi + \eta} \left[ \frac{\partial}{\partial \xi} \left( \xi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \eta \frac{\partial}{\partial \eta} \right) \right] + \frac{1}{\xi\eta} \frac{\partial^2}{\partial \phi^2} \right\} \psi_c + \frac{2Z_1 Z_2 e^2}{\xi + \eta} \psi_c = E \psi_c. \quad (6.6)$$

Since we are interested in a scattering solution  $\psi_c$  which exhibits azimuthal symmetry, we write

$$\psi_c = f(\xi)g(\eta) \quad (6.7)$$

and separate the Schrödinger equation (6.6) to obtain the two differential equations

$$\frac{d}{d\xi} \left( \xi \frac{df}{d\xi} \right) + (\frac{1}{4}k^2\xi - v_1)f = 0 \quad (6.8a)$$

$$\frac{d}{d\eta} \left( \eta \frac{dg}{d\eta} \right) + (\frac{1}{4}k^2\eta - v_2)g = 0. \quad (6.8b)$$

The two separation constants  $v_1$  and  $v_2$  are such that

$$v_1 + v_2 = \gamma k \quad (6.9)$$

where we have defined the quantity

$$\gamma = mZ_1Z_2e^2/\hbar^2k = Z_1Z_2e^2/\hbar v \quad (6.10)$$

and we recall that  $v = \hbar k/m$  is the magnitude of the relative velocity.

In order to determine the two functions  $f(\xi)$  and  $g(\eta)$ , we first notice that

$$\exp(ikz) = \exp\{\frac{1}{2}ik(\xi - \eta)\}$$

while

$$\exp(ikr) = \exp\{\frac{1}{2}ik(\xi + \eta)\}.$$

This suggests that we choose

$$f(\xi) = \exp(\frac{1}{2}ik\xi) \quad (6.11)$$

which indeed is a solution of eq. (6.8a) provided that  $v_1 = \frac{1}{2}ik$ . With the help of eq. (6.9) we may then rewrite eq. (6.8b) as

$$\frac{d}{d\eta}\left(\eta \frac{dg}{d\eta}\right) + \frac{1}{4}k^2\eta g - (\gamma k - \frac{1}{2}ik)g = 0. \quad (6.12)$$

Let us define a new function  $h(\eta)$  by the relation

$$g(\eta) = \exp\{-\frac{1}{2}ik\eta\}h(\eta). \quad (6.13)$$

Substituting this expression for  $g(\eta)$  in eq. (6.12), we obtain

$$\eta \frac{d^2h}{d\eta^2} + (1 - ik\eta) \frac{dh}{d\eta} - \gamma kh = 0. \quad (6.14)$$

This last equation can be identified with the Kummer–Laplace differential equation

$$z \frac{d^2w}{dz^2} + (c - z) \frac{dw}{dz} - aw = 0 \quad (6.15)$$

whose solution, regular at the origin  $z = 0$ , is the confluent hypergeometric function  ${}_1F_1(a; c; z)$ . Thus we find that

$$h(\eta) = C {}_1F_1(-i\gamma; 1; ik\eta) \quad (6.16)$$

where  $C$  is a constant. Hence the Schrödinger equation (6.6) admits the regular solution

$$\psi_c = C e^{ikz} {}_1F_1(-i\gamma; 1; ik(r - z)). \quad (6.17)$$

Before we analyze the asymptotic behaviour of the function  $\psi_c$ , let us study in more detail the solutions of the Kummer–Laplace equation (6.15). The confluent hypergeometric function  ${}_1F_1(a; c; z)$  can be written as a power series

$$\begin{aligned} {}_1F_1(a; c; z) &= 1 + \frac{a}{c} \frac{z}{1!} + \frac{a(a+1)}{c(c+1)} \frac{z^2}{2!} + \cdots \\ &= \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(c)}{\Gamma(a)\Gamma(c+n)} \frac{z^n}{n!} \end{aligned} \quad (6.18)$$

where  $\Gamma$  is Euler's gamma function.

Except for the case  $c = -p$  ( $p$  integer  $\geq 0$ ), the series (6.18) defines an entire function of  $z$ . It clearly reduces to a polynomial of degree  $p$  if  $a = -p$ , and exhibits an essential singularity at infinity if  $a \neq -p$ . For the case where  $a$  is not an integer and  $c$  is an integer  $> 0$ , which is of interest to us [see eq. (6.16)] one can use the following integral representation of  ${}_1F_1(a; c; z)$  [6]

$${}_1F_1(a; c; z) = (1 - e^{-2\pi ia})^{-1} \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \oint_C e^{zt} t^{a-1} (1-t)^{c-a-1} dt. \quad (6.19)$$

Here  $C$  is a simple loop in the complex  $t$ -plane enclosing the points  $t = 0$  and  $t = 1$  where the integrand has branch points, and we have chosen the cut to join these points (see Fig. 6.1)

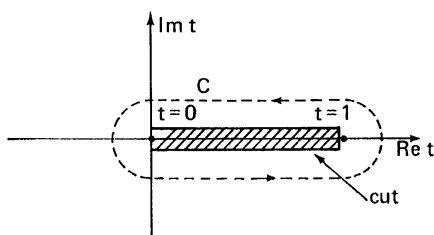


Fig. 6.1. The integration contour used in eq. (6.19) to obtain the function  ${}_1F_1(a; c; z)$ .

If the cuts are drawn as shown on Fig. 6.2 and the contour  $C$  in eq. (6.19) is replaced respectively by the integration paths  $C_1$  and  $C_2$  (i.e. loops coming from  $i\infty$  and enclosing one of the branch points in the positive sense) one obtains successively two linearly independent solutions, irregular at the origin,

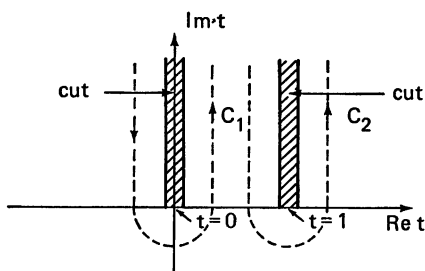


Fig. 6.2. The integration paths  $C_1$  and  $C_2$  which correspond respectively to the functions  $W_1(a; c; z)$  and  $W_2(a; c; z)$ .

called  $W_1(a; c; z)$  and  $W_2(a; c; z)$  [6]. In terms of these functions, the solution of eq. (6.15), regular at  $z = 0$ , can be written as

$${}_1F_1(a; c; z) = W_1(a; c; z) + W_2(a; c; z). \quad (6.20)$$

It is also convenient to introduce another solution of eq. (6.15), irregular at the origin, as

$$G(a; c; z) = -i[W_1(a; c; z) - W_2(a; c; z)]. \quad (6.21)$$

The solutions  $W_1(a; c; z)$  and  $W_2(a; c; z)$  have simple asymptotic (semi-convergent) expansions, namely [e.g. 6]

$$W_1(a; c; z)|_{|z| \rightarrow \infty} \approx \frac{\Gamma(c)}{\Gamma(c-a)} (-z)^{-a} v(a; a-c+1; -z),$$

$$-\pi < \arg(-z) < +\pi \quad (6.22)$$

and

$$W_2(a; c; z)|_{|z| \rightarrow \infty} \approx \frac{\Gamma(c)}{\Gamma(a)} e^z z^{a-c} v(1-a; c-a; z),$$

$$-\pi < \arg z < +\pi \quad (6.23)$$

where

$$v(\alpha; \beta; z) = 1 + \frac{\alpha\beta}{1!z} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{2!z^2} + \dots$$

$$= \sum_{n=0}^{\infty} \frac{\Gamma(n+\alpha)\Gamma(n+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{(z)^{-n}}{n!}. \quad (6.24)$$

We are now ready to obtain the asymptotic form of the function  $\psi_c$ . Using eq. (6.20), we first rewrite the relation (6.17) as

$$\psi_c = C[\psi_1 + \psi_2] \quad (6.25)$$

where

$$\psi_1 = e^{ikz} W_1(-i\gamma; 1; ik(r-z)) \quad (6.26)$$

and

$$\psi_2 = e^{ikz} W_2(-i\gamma; 1; ik(r-z)). \quad (6.27)$$

The asymptotic expansions (6.22)–(6.24) then yield

$$\psi_1 \xrightarrow{|r-z| \rightarrow \infty} \frac{\exp(\frac{1}{2}\pi\gamma)}{\Gamma(1+i\gamma)} \exp\{i[kz + \gamma \log k(r-z)]\} \left[ 1 + \frac{\gamma^2}{ik(r-z)} + \dots \right] \quad (6.28)$$

and

$$\psi_2 \xrightarrow{|r-z| \rightarrow \infty} \frac{\exp(\frac{1}{2}\pi\gamma)}{\Gamma(-i\gamma)} \frac{\exp\{i[kr - \gamma \log k(r-z)]\}}{ik(r-z)} \left[ 1 + \frac{(1+i\gamma)^2}{ik(r-z)} + \dots \right] \quad (6.29)$$

where we have used the fact that the purely imaginary variable  $u = ik(r-z)$  can be written as  $u = \exp\{\log|u|\} \exp\{\frac{1}{2}i\pi\}$ . Since  $t\Gamma(t) = \Gamma(t+1)$  so that  $\Gamma(-i\gamma) = \Gamma(1-i\gamma)/(-i\gamma)$  we may rewrite the relation (6.29) as

$$\psi_2 \xrightarrow{|r-z| \rightarrow \infty} -\frac{\gamma \exp\{\frac{1}{2}\pi\gamma\}}{\Gamma(1-i\gamma)} \frac{\exp\{i[kr - \gamma \log k(r-z)]\}}{k(r-z)} \times \left[ 1 + \frac{(1+i\gamma)^2}{ik(r-z)} + \dots \right]. \quad (6.30)$$

Using eqs. (6.25), (6.28) and (6.30) together with the fact that  $z = r \cos \theta$ , we find that

$$\psi_c \xrightarrow{|r-z| \rightarrow \infty} C \frac{\exp(\frac{1}{2}\pi\gamma)}{\Gamma(1+i\gamma)} \left[ \exp\{i[kz + \gamma \log kr(1 - \cos\theta)]\} \left( 1 + \frac{\gamma^2}{ikr(1 - \cos\theta)} + \dots \right) + f_c(\theta) \frac{\exp\{i(kr - \gamma \log 2kr)\}}{r} \left( 1 + \frac{(1+i\gamma)^2}{ikr(1 - \cos\theta)} + \dots \right) \right] \quad (6.31)$$

where

$$f_c(\theta) = -\gamma \exp(2i\sigma_0) \frac{\exp\{-i\gamma \log(\sin^2 \frac{1}{2}\theta)\}}{2k \sin^2 \frac{1}{2}\theta} \quad (6.32)$$

and

$$\exp(2i\sigma_0) = \Gamma(1+i\gamma)/\Gamma(1-i\gamma) \quad (6.33)$$

so that

$$\sigma_0 = \arg \Gamma(1+i\gamma). \quad (6.34)$$

Clearly, the relation (6.31) does not hold for  $\theta = 0$ , in which case  $z = r$  and we cannot let  $|r - z|$  tend to infinity.

Let us now compare the asymptotic behaviour of the Coulomb wave function  $\psi_c$  [see eq. (6.31)] with that of the stationary scattering wave function  $\psi_{k_1}^{(+)}$  corresponding to a potential of finite range, namely

$$\psi_{k_1}^{(+)} \xrightarrow{r \rightarrow \infty} A \left[ e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r} \right]. \quad (6.35)$$

We see that the asymptotic form of  $\psi_c$  does not reduce to the simple expression (6.35). The long range character of the Coulomb force prevents the first term on the right of eq. (6.31) from approaching a plane wave, while the second term does not exhibit the simple form  $\exp(ikr)/r$ . However, when  $|r - z| \rightarrow \infty$  the modifications due to the Coulomb interaction only affect the *phases* of these terms, so that the two terms on the right of eq. (6.31) can again be interpreted respectively as an incident wave and an outgoing scattered wave. Indeed, if we calculate the probability current density at large  $r$  – ignoring the interference term since we stay away from  $\theta = 0$  [7] – the first term of eq. (6.31) yields a probability current  $j_{inc}$  such that the incident flux through a unit area normal to the incident wave vector  $k_1$  is given by

$$j_{inc} \cdot k_1 = B^* B |v| \quad (6.36)$$

where

$$B = C \exp\{\frac{1}{2}\pi\gamma\}/\Gamma(1+i\gamma) \quad (6.37)$$

and we remark that the logarithmic phase gives a correction of order  $r^{-1}$  which can be neglected.

Similarly, the current density  $j_{out}$  calculated for large  $r$  from the second term on the right of eq. (6.31) is directed radially and is such that the outgoing flux through a unit area normal to  $\hat{r}$  is given by

$$j_{out} \cdot \hat{r} = B^* B v \frac{1}{r^2} |f_c(\theta)|^2, \quad (6.38)$$

the effect due to the presence of the factor  $\exp[-i\gamma \log(2kr)]$  being negligible to lowest order in  $r^{-1}$ .

Taking the ratio of the scattered flux into the solid angle  $(\Omega, \Omega + d\Omega)$  to the incident flux, we find that the differential Coulomb scattering cross section is simply [8]

$$d\sigma_c/d\Omega = |f_c|^2 \quad (6.39)$$

or

$$\frac{d\sigma_c}{d\Omega} = \frac{\gamma^2}{4k^2 \sin^4 \frac{1}{2}\theta} = \left\{ \frac{Z_1 Z_2 e^2}{4E \sin^2 \frac{1}{2}\theta} \right\}^2, \quad (6.40)$$

We note that eq. (6.40), which does not involve Planck's constant  $\hbar$ , is identical to the *Rutherford formula* derived by Rutherford [9] from classical mechanics. Although the angle dependent part occurring in the *phase* of the scattering amplitude  $f_c(\theta)$  has clearly no effect on the Coulomb differential cross section (6.40), we shall see in Chapter 7 that it leads to non-classical effects when the colliding particles are identical.

There are other remarkable features of Coulomb scattering contained in the Rutherford formula (6.40). The differential cross section  $d\sigma_c/d\Omega$  does *not* depend on the *sign* of the potential. Also, since the energy and the scattering angle  $\theta$  enter into separate multiplicative factors, the angular distribution is independent of the energy [10]. Moreover, at fixed  $\theta$ , the cross section is proportional to  $E^{-2}$ . Finally, the quantity  $d\sigma_c/d\Omega$  is infinite in the forward direction ( $\theta = 0$ ) and the total cross section is also infinite, since the expression  $\int (d\sigma_c/d\Omega) d\Omega$  diverges at  $\theta = 0$ . However, as we remarked at the beginning of this chapter, the Coulomb field is screened by other charges in actual physical situations at a distance  $R_s$ . The expressions (6.32) and (6.40) are therefore correct only for momentum transfers  $2\hbar k \sin \frac{1}{2}\theta$  large with respect to  $\hbar/R_s$ , and there is no cause for alarm in the fact that the pure Coulomb total cross section is infinite.

Incidentally, it is of interest to mention at this point an important difference between classical and quantum scattering. In classical theory, the total cross section always fails to exist if the forces have an infinite range, no matter how fast they tend to zero. This is due to the fact that two classical particles interacting through forces of infinite range always suffer some deflection, even if they pass by each other at an arbitrary large distance (i.e. at a large impact parameter). Hence, for such interactions, the classical differential cross section is always infinite for  $\theta = 0$ , and the total classical cross section is also infinite. On the contrary, in quantum mechanics, it is a simple matter to show that the total cross section remains finite if the potential decreases faster than  $r^{-2}$  for large  $r$ , while the differential cross section at  $\theta = 0$  remains finite if the interaction decreases faster than  $r^{-3}$  (see Problem II, 14).

Let us now return to the Coulomb scattering wave function  $\psi_c$  whose asymptotic behaviour is given by eq. (6.31). In what follows we shall adopt a

“normalization” convention similar to that discussed in Section 5.1 and leading to the expression

$$\psi_{k_1}^{(+)} \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} [e^{ikz} + f(\theta, \phi) e^{ikr/r}] \quad (6.41)$$

for potentials of finite “range”. Thus, normalizing the incident wave so that it gives a probability density  $(2\pi)^{-3}$  in configuration space, we find from eq. (6.31) that

$$C = (2\pi)^{-3/2} \exp(-\frac{1}{2}\pi\gamma)\Gamma(1 + i\gamma). \quad (6.42)$$

Hence the Coulomb wave function (6.17) becomes

$$\psi_c = (2\pi)^{-3/2} \exp(-\frac{1}{2}\pi\gamma)\Gamma(1 + i\gamma) e^{ikz} {}_1F_1(-i\gamma; 1; ik(r - z)) \quad (6.43)$$

and

$$\begin{aligned} \psi_c \xrightarrow{|r-z| \rightarrow \infty} (2\pi)^{-3/2} & \left[ \exp\{i[kz + \gamma \log kr(1 - \cos \theta)]\} \left( 1 + \frac{\gamma^2}{ikr(1 - \cos \theta)} + \dots \right) \right. \\ & \left. + f_c(\theta) \frac{\exp\{i(kr - \gamma \log 2kr)\}}{r} \left( 1 + \frac{(1+i\gamma)^2}{ikr(1 - \cos \theta)} + \dots \right) \right]. \end{aligned} \quad (6.44)$$

We note that the probability of finding the particle at  $r = 0$  relative to that of finding it in the incident beam is given by

$$|\psi_c(0)|^2/|\psi_c(\infty)|^2 = e^{-\pi\gamma} |\Gamma(1 + i\gamma)|^2 = 2\pi\gamma/(e^{2\pi\gamma} - 1) \quad (6.45)$$

where we have used eq. (6.18) to obtain  $\psi_c(0)$ . If the Coulomb potential is repulsive ( $\gamma > 0$ ) and strong compared with the kinetic energy of the particle, so that  $\gamma \gg 1$ , we have

$$|\psi_c(0)|^2/|\psi_c(\infty)|^2 \simeq 2\pi\gamma \exp(-2\pi\gamma). \quad (6.46)$$

The quantity  $\exp(-2\pi\gamma) = \exp(-2\pi Z_1 Z_2 e^2/\hbar v)$  is called the Gamow factor [11]. It plays an important role in the description of reactions between positively charged nuclei at low relative velocities, as well as in the theory of alpha decay.

Let us now examine briefly *shielding effects*, assuming that the pure Coulomb potential (6.1) is replaced by the screened potential (6.2), with the screening function  $s(r)$  given by eq. (6.3). Comparing the asymptotic behaviour (6.44) of the Coulomb wave function with the corresponding expression (6.41) valid for the screened potential, we see that if

$$\gamma^2/k \ll R_s(1 - \cos \theta) \quad (6.47)$$

then the screened potential scattering amplitude  $f(\theta)$  differs from  $f_c(\theta)$  only by a logarithmic phase factor, namely

$$f(\theta) = f_c(\theta) \exp\{-i\gamma \log 2kR_s\} \quad (6.48)$$

and the differential cross section is unchanged by the screening. For scattering angles

$$\theta < \gamma/(kR_s)^{1/2} \quad (6.49)$$



which do not obey the condition (6.47), the terms of order  $R_s^{-1}$  in eq. (6.44) must be taken into account. In many nuclear and elementary particle processes [where the screening function (6.3) is used] the angular range defined by eq. (6.49) is small compared with the acceptance angle of the detectors [12].

## 6.2. Partial wave decomposition

We shall now solve the problem of Coulomb scattering in spherical polar coordinates, using the method of partial waves. This way of approaching the problem is not of great interest for pure Coulomb scattering, since the treatment in parabolic coordinates is simpler. In addition, because the Coulomb interaction drops off so slowly for large  $r$ , we expect the partial wave expansion for the scattering amplitude  $f_c(\theta)$  to be of little use. However, the partial wave decomposition is essential for the study of scattering problems where a short-range potential is added to the pure Coulomb interaction. This situation arises for example in proton-proton scattering, where departures from the Coulomb potential occur at small distances, due to the short range, strong interaction between the two colliding protons. We shall study the problem of treating the superposition of a Coulomb and a short-range potential in Section 6.3. Returning now to pure Coulomb scattering in spherical polar coordinates, we write the Schrödinger equation as

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right] \psi + \frac{Z_1 Z_2 e^2}{r} \psi = E \psi \quad (6.50)$$

where the operator  $L^2$  is given by eq. (4.6). Let us expand the wave function  $\psi$  in partial waves as

$$\psi = r^{-1} \sum_{l=0}^{\infty} w_l(k, r) P_l(\cos \theta) \quad (6.51)$$

so that the radial functions  $w_l(k, r)$  satisfy the equation

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - 2\gamma k/r] w_l(k, r) = 0 \quad (6.52)$$

where  $\gamma$  is defined in eq. (6.10). If we now substitute

$$w_l(k, r) = e^{ikr} (kr)^{l+1} f_l(\alpha r) \quad (6.53)$$

and set  $\xi = \alpha r$ , we find that the function  $f_l(\xi)$  satisfies the Kummer-Laplace equation

$$\xi d^2 f_l / d\xi^2 + (2l + 2 - \xi) df_l / d\xi - (l + 1 + i\gamma) f_l = 0 \quad (6.54)$$

if we choose  $\alpha = -2ik$ . Therefore the solution of this equation, regular at  $r = 0$  is

$$f_l = C_l {}_1F_1(l + 1 + i\gamma; 2l + 2; -2ikr) \quad (6.55)$$

and the *regular spherical Coulomb function*  $F_l(k, r)$  obtained by substituting the regular solution (6.55) in eq. (6.53) is then

$$F_l(k, r) = C_l e^{ikr} (kr)^{l+1} {}_1F_1(l+1+i\gamma; 2l+2; -2ikr). \quad (6.56)$$

The asymptotic form of  $F_l(k, r)$  may be found from the semi-convergent expansions (6.22)–(6.24). This yields

$$F_l(k, r) \xrightarrow{r \rightarrow \infty} C_l \frac{\exp\{\frac{1}{2}\pi\gamma + i\sigma_l\} (2l+1)!}{2^l \Gamma(l+1+i\gamma)} \sin(kr - \frac{1}{2}l\pi - \gamma \log 2kr + \sigma_l) \quad (6.57)$$

where [compare with eq. (4.44)] the quantity

$$\sigma_l = \arg \Gamma(l+1+i\gamma) \quad (6.58)$$

is called the *Coulomb phase shift*. Hence the “*Coulomb S-matrix element*”, defined by analogy with the *S-matrix element* of eq. (4.50), is given by

$$S_l^c(k) = \exp\{2i\sigma_l(k)\} = \Gamma(l+1+i\gamma)/\Gamma(l+1-i\gamma). \quad (6.59)$$

If we require by analogy with eq. (4.84a) that

$$F_l(k, r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi - \gamma \log 2kr + \sigma_l) \quad (6.60)$$

then the quantities  $C_l$  are such that

$$\begin{aligned} C_l &= \frac{2^l \exp(-\frac{1}{2}\pi\gamma) |\Gamma(l+1+i\gamma)|}{(2l+1)!} \\ &= C_0 \frac{2^l}{(2l+1)!} [(l^2 + \gamma^2)[(l-1)^2 + \gamma^2] \dots (1 + \gamma^2)]^{1/2} \end{aligned} \quad (6.61)$$

with

$$C_0 = [2\pi\gamma/(e^{2\pi\gamma} - 1)]^{1/2}. \quad (6.62)$$

Hence

$$\begin{aligned} F_l(k, r) &= \frac{2^l \exp(-\frac{1}{2}\pi\gamma) |\Gamma(l+1+i\gamma)|}{(2l+1)!} e^{ikr} (kr)^{l+1} \\ &\quad \times {}_1F_1(l+1+i\gamma; 2l+2; -2ikr). \end{aligned} \quad (6.63)$$

It is easily verified that with the choice  $w_l = F_l$ , the function  $\psi$  of eq. (6.51) is proportional to the Coulomb scattering wave function  $\psi_c$  which we have calculated above in parabolic coordinates. If we adopt the “normalization” leading to the asymptotic behaviour (6.44) we find that

$$\begin{aligned} \psi_c &= (2\pi)^{-3/2} \exp(-\frac{1}{2}\pi\gamma) \Gamma(1+i\gamma) e^{ikz} {}_1F_1(-i\gamma; 1; ik(r-z)) \\ &= \sum_{l=0}^{\infty} \tilde{C}_l e^{ikr} k^{l+1} r^l {}_1F_1(l+1+i\gamma; 2l+2; -2ikr) P_l(\cos \theta). \end{aligned} \quad (6.64)$$

The new coefficients  $\tilde{C}_l$  may be obtained by using the orthogonality property of the Legendre polynomials and matching the two sides of eq. (6.64) at  $r = 0$ . One finds

$$\tilde{C}_l = (2\pi)^{-3/2} k^{-1} (2l+1) i^l \exp(i\sigma_l) C_l \quad (6.65)$$

so that

$$\psi_c = (2\pi)^{-3/2} (kr)^{-1} \sum_{l=0}^{\infty} (2l+1)! \exp(i\sigma_l) F_l(k, r) P_l(\cos \theta) \quad (6.66)$$

with  $F_l(k, r)$  given by eq. (6.63). This development bears a strong resemblance to that of the plane wave

$$\Phi_{k_i} = (2\pi)^{-3/2} \exp(ik_i \cdot r) = (2\pi)^{-3/2} \sum_{l=0}^{\infty} (2l+1)! j_l(kr) P_l(\cos \theta) \quad (6.67)$$

to which it reduces when  $\gamma \rightarrow 0$ .

One can also obtain *irregular* spherical Coulomb functions by looking for solutions of eq. (6.54) which are irregular at the origin. In terms of the two irregular solutions  $W_1$  and  $W_2$  introduced in Section 6.1, one may define the irregular spherical Coulomb functions

$$G_l(k, r) = -iC_l e^{ikr} (kr)^{l+1} [W_1(l+1+i\gamma; 2l+2; -2ikr) - W_2(l+1+i\gamma; 2l+2; -2ikr)], \quad (6.68)$$

and

$$\begin{aligned} H_l^{(\pm)}(k, r) &= 2C_l \exp(\mp i\sigma_l) e^{\pm ikr} (kr)^{l+1} W_1(l+1 \pm i\gamma; 2l+2; \mp 2ikr) \\ &= 2C_l \exp(\mp i\sigma_l) e^{\mp ikr} (kr)^{l+1} W_2(l+1 \mp i\gamma; 2l+2; \pm 2ikr). \end{aligned} \quad (6.69)$$

With the choice (6.61) for the quantities  $C_l$ , these functions have the following asymptotic forms:

$$G_l(k, r) \xrightarrow{r \rightarrow \infty} -\cos(kr - \frac{1}{2}l\pi - \gamma \log 2kr + \sigma_l) \quad (6.70)$$

and

$$H_l^{(\pm)}(k, r) \xrightarrow{r \rightarrow \infty} \mp i \exp\{\pm i(kr - \frac{1}{2}l\pi - \gamma \log 2kr)\}. \quad (6.71)$$

The functions  $F_l$  and  $G_l$  are real, while  $H_l^{(+)}$  and  $H_l^{(-)}$ , which behave respectively as pure outgoing and incoming waves for large values of  $r$ , are such that  $H_l^{(-)} = H_l^{(+)*}$ . We also have

$$F_l = \frac{1}{2}\{H_l^{(+)} \exp(i\sigma_l) + H_l^{(-)} \exp(-i\sigma_l)\}, \quad (6.72)$$

$$G_l = \frac{1}{2i}\{H_l^{(+)} \exp(i\sigma_l) - H_l^{(-)} \exp(-i\sigma_l)\}$$

and

$$H_l^{(\pm)} = \exp(\mp i\sigma_l) \{F_l \pm iG_l\}.$$

In terms of the functions  $H_l^{(+)}$  and  $H_l^{(-)}$ , eq. (6.66) can be rewritten as

$$\begin{aligned} \psi_c &= (2\pi)^{-3/2} (2kr)^{-1} \sum_{l=0}^{\infty} (2l+1)! \\ &\times [H_l^{(-)}(k, r) + \exp(2i\sigma_l) H_l^{(+)}(k, r)] P_l(\cos \theta). \end{aligned} \quad (6.73)$$

Returning to eq. (6.56), we note that near  $kr = 0$  we may develop  $\exp(ikr) = 1 + ikr - \frac{1}{2}(kr)^2 + \dots$  and also retain the first few terms in the expansion (6.18) of the confluent hypergeometric function to obtain

$$F_l = C_l(kr)^{l+1} \left[ 1 + ikr - \frac{1}{2}k^2r^2 + \dots \right] \left[ 1 - \frac{l+1+i\gamma}{2l+2} 2ikr - \frac{(l+1+i\gamma)(l+2+i\gamma)}{(2l+2)(2l+3)} \frac{4k^2r^2}{2} + \dots \right] \\ = C_l(kr)^{l+1} \left\{ 1 + \frac{\gamma}{l+1}kr + \frac{2\gamma^2 - l - 1}{(2l+2)(2l+3)}k^2r^2 + \dots \right\} \quad (6.74)$$

and in particular for  $l = 0$

$$F_0 = C_0kr[1 + \gamma kr + (\frac{1}{3}\gamma^2 - \frac{1}{6})k^2r^2 + \dots]. \quad (6.75)$$

The corresponding expansions for  $G_l$  near  $kr = 0$  are

$$G_l = -[(2l+1)C_l]^{-1}(kr)^{-l}[1 + \mathcal{O}(\gamma kr/l)], \quad l \neq 0 \quad (6.76)$$

and

$$G_0 = -C_0^{-1} \{ 1 + 2kr\gamma[\log(2kr) + 2\hat{C} - 1 + h(\gamma) + \log \gamma] + (3\gamma^2 - \frac{1}{2})k^2r^2 + \dots \} \quad (6.77)$$

where

$$h(\gamma) + \log \gamma = \gamma^2 \sum_{s=1}^{\infty} \frac{1}{s(s^2 + \gamma^2)} - \hat{C} \quad (6.78)$$

and  $\hat{C} = 0.577215$  is Euler's constant.

Finally, for  $\gamma = 0$ , the functions  $F_l$ ,  $G_l$  and  $H_l^{(\pm)}$  reduce (within a factor  $\rho = kr$ ) to the spherical Bessel functions introduced previously (see Section 4.1) in connection with the radial equation of a free particle. That is

$$F_l(\gamma = 0, \rho) = \rho j_l(\rho), \\ G_l(\gamma = 0, \rho) = \rho n_l(\rho), \\ H_l^{(+)}(\gamma = 0, \rho) = \rho h_l^{(1)}(\rho) \quad (6.79)$$

and

$$H_l^{(-)}(\gamma = 0, \rho) = \rho h_l^{(2)}(\rho).$$

Additional properties of the spherical Coulomb functions may be found for example in the references [5] and [13].

### 6.3. Scattering by a modified Coulomb field

Consider now the situation where a short-range potential  $V(r) = \hbar^2 U(r)/2m$  is added to the Coulomb field  $V_c(r)$ . We expand the wave function as

$$\psi = r^{-1} \sum_{l=0}^{\infty} \chi_l(k, r) P_l(\cos \theta) \quad (6.80)$$

and find that the radial wave equation for the functions  $\chi_l$  reads

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{2\gamma k}{r} - U(r) - \frac{l(l+1)}{r^2} \right] \chi_l(k, r) = 0, \quad (6.81)$$

with

$$\chi_l(k, r) \underset{r \rightarrow 0}{\sim} r^{l+1}. \quad (6.82)$$

As  $r \rightarrow \infty$ , the Coulomb field dominates the terms  $U(r)$  and  $l(l+1)/r^2$  so that the functions  $\chi_l$  approach linear combinations of spherical Coulomb functions. Since the actual interaction departs from the Coulomb form at small values of  $r$ , the regular solution of eq. (6.81) is now allowed to contain some admixture of the irregular solution  $G_l$  of eq. (6.52). Thus we have

$$\chi_l(k, r) \underset{r \rightarrow \infty}{\rightarrow} B_l^{(1)}(k) F_l(k, r) + B_l^{(2)}(k) G_l(k, r) \quad (6.83)$$

where  $B_l^{(1)}$  and  $B_l^{(2)}$  are two "constants" (for fixed  $k$ ). It is convenient to rewrite this relation in terms of the functions  $H_l^{(+)}$  and  $H_l^{(-)}$  defined by eq. (6.69). Thus

$$\chi_l \underset{r \rightarrow \infty}{\rightarrow} A_l [H_l^{(-)}(k, r) + \exp(2i\Delta_l) H_l^{(+)}(k, r)] \quad (6.84)$$

or

$$\begin{aligned} \chi_l(r) \underset{r \rightarrow \infty}{\rightarrow} \tilde{A}_l \{ \exp\{ -i[kr - \tfrac{1}{2}l\pi - \gamma \log 2kr] \} \\ - \exp(2i\Delta_l) \exp\{ i[kr - \tfrac{1}{2}l\pi - \gamma \log 2kr] \} \} \end{aligned} \quad (6.85)$$

where  $A_l$  and  $\tilde{A}_l = iA_l$  are "normalization" constants and we have used the asymptotic forms (6.71) of the functions  $H_l^{(\pm)}$ . If the short-range potential is real the quantity  $\Delta_l$  is easily seen to be also real from probability conservation. Since  $\Delta_l = \sigma_l$  when  $V = 0$ , we set

$$\Delta_l = \sigma_l + \delta_l \quad (6.86)$$

where the additional phase shift  $\delta_l$  is the phase shift due to the extra potential  $V$  in the presence of the Coulomb potential  $V_c$ . It is important to note that this phase shift is not the same as the one which would be obtained from  $V$  alone.

The calculation of  $\delta_l$  from the radial equation (6.81) follows from a simple adaptation of the reasoning given in Section 4.3.2. One finds (see in particular eq. (4.113') in footnote [26] of Chapter 4) that

$$\tan \delta_l(k) = \frac{kF'_l(ka) - \hat{\alpha}_l(k)F_l(ka)}{kG'_l(ka) - \hat{\alpha}_l(k)G_l(ka)} \quad (6.87)$$

where the logarithmic derivative

$$\hat{\alpha}_l(k) = [\chi_l^{-1}(d\chi_l/dr)]_{r=a} \quad (6.88)$$

is in general obtained after a numerical integration of the radial Schrödinger equation (6.81) in the interior region has yielded the wave function  $\chi_l(k, r)$  and its first derivative at  $r = a$ .

The constants  $A_l$  appearing in eq. (6.84) can be determined by requiring that the function  $\psi$  behaves asymptotically as a Coulomb wave  $\psi_c$  plus an extra outgoing wave in  $\exp[i(kr - \gamma \log 2kr)]/r$ . Thus, if we choose the normalization (6.44) for  $\psi_c$ , we find that

$$A_l = (2\pi)^{-3/2} k^{-1} (2l+1) i^l \quad (6.89)$$

so that

$$\begin{aligned} \psi \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} (2kr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^l \\ \times [H_l^{(-)}(k, r) + \exp\{2i(\sigma_l + \delta_l)\} H_l^{(+)}(k, r)] P_l(\cos \theta). \end{aligned} \quad (6.90)$$

Comparing this result with eq. (6.73), we deduce that

$$\begin{aligned} \psi \xrightarrow{r \rightarrow \infty} \psi_c + (2\pi)^{-3/2} (2kr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^l \exp(2i\sigma_l) \\ \times \{\exp(2i\delta_l) - 1\} H_l^{(+)}(k, r) P_l(\cos \theta). \end{aligned} \quad (6.91)$$

The scattering amplitude  $f(\theta)$  associated with the outgoing spherical wave of  $\psi$  is then found to be

$$f(\theta) = f_c(\theta) + \hat{f}(\theta) \quad (6.92)$$

where  $f_c(\theta)$  is the Coulomb scattering amplitude given by eq. (6.32) and

$$\hat{f}(\theta) = (2ik)^{-1} \sum_{l=0}^{\infty} (2l+1) \exp(2i\sigma_l) \{\exp(2i\delta_l) - 1\} P_l(\cos \theta). \quad (6.93)$$

The series (6.93) converges more rapidly the lower the bombarding energies and (or) the shorter the range of the potential  $V$ .

The differential scattering cross section is

$$d\sigma/d\Omega = |f(\theta)|^2 \quad (6.94)$$

and can be written as

$$d\sigma/d\Omega = |f_c(\theta)|^2 + |\hat{f}(\theta)|^2 + 2 \operatorname{Re}[f_c^*(\theta) \hat{f}(\theta)] \quad (6.95)$$

so that it contains an interference term between the Coulomb amplitude  $f_c(\theta)$  and the amplitude  $\hat{f}(\theta)$ . The analysis leading to eq. (6.95) plays an important role in the interpretation of many nuclear reactions. For example, with the appropriate modifications to account for identical particles [14] it has been used to study nuclear forces [e.g. 15] in low-energy proton-proton scattering.

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# The Scattering of Identical Particles

Two particles are said to be identical when they cannot be distinguished by means of any intrinsic property. This indistinguishability of identical particles leads to profound consequences in quantum mechanics. In particular, the treatment of the scattering problem must be modified to analyze collisions involving identical particles. We first outline in Section 7.1 the content of the symmetrization postulate and the classification of particles into bosons and fermions. Boson–boson scattering is examined in Section 7.2, while Section 7.3 deals with fermion–fermion scattering. In both cases the non-classical effects due to the indistinguishability of the colliding particles are analyzed, with particular attention to the case of Coulomb scattering.

## *7.1. The symmetrization postulate. Bosons and fermions*

We first note that in quantum mechanics there is no way of keeping track of each particle individually when the wave functions of two identical particles overlap. Therefore it is impossible to distinguish between identical particles in regions of space where they may be found simultaneously, such as their interaction region. This difficulty does not arise in classical mechanics. Indeed, the existence of sharp trajectories makes it possible in principle to distinguish classical particles by their paths. Even if we are not always able in practice to follow classical particles along their trajectories, so that an ambiguity in the initial conditions of the motion of two classical particles arises, the laws of motion remain the same so that the labelling of the trajectories is merely a question of convention; it has no effect on physical phenomena.



Let us now study a quantum mechanical system of  $N$  identical particles. The basic dynamical variables of the  $i$ th particle are its position  $\mathbf{r}_i$ , momentum  $\mathbf{p}_i$  and spin or intrinsic angular momentum  $s_i$ , so that the particles here may be thought of as “elementary” [1]. Let  $q_i$  be a complete set of commuting observables for the particle  $i$ , for example its position  $\mathbf{r}_i$  and the third component of its spin  $s_{zi}$ . Since the  $N$  particles are identical, all observables corresponding to this system must be symmetric functions of the basic dynamical variables. For example, the Hamiltonian  $H$  must be symmetric in the interchange of any pair of particles  $i$  and  $j$ . Specifically, an interchange operator  $P_{ij}$  that permutes the variables  $q_i$  and  $q_j$  of particles  $i$  and  $j$  commutes with the Hamiltonian

$$[P_{ij}, H] = 0. \quad (7.1)$$

Since two successive interchanges of  $q_i$  and  $q_j$  bring the particles back to their initial configurations, we have

$$P_{ij}^2 = I \quad (7.2)$$

so that the eigenvalues of the interchange operator  $P_{ij}$  are  $\pm 1$ .

More generally, there are  $N!$  different permutations of the  $N$  variables  $q_1, \dots, q_N$ . If we define  $P$  as the permutation that replaces  $q_1$  by  $q_{P1}$ ,  $q_2$  by  $q_{P2}$ ,  $\dots$ ,  $q_N$  by  $q_{PN}$  and since  $P$  can be obtained as a succession of interchanges, we have

$$[P, H] = 0. \quad (7.3)$$

A permutation  $P$  is said to be *even* or *odd* depending on whether the number of interchanges leading to it is even or odd.

If we let the operator  $P_{ij}$  act on a wave function  $\psi(q_1, q_2, \dots, q_N)$ , we have

$$P_{ij}\psi(q_1, \dots, q_i, \dots, q_j, \dots, q_N) = \psi(q_1, \dots, q_j, \dots, q_i, \dots, q_N) \quad (7.4)$$

and for the general permutation

$$P\psi(q_1, q_2, \dots, q_N) = \psi(q_{P1}, q_{P2}, \dots, q_{PN}). \quad (7.5)$$

The  $N!$  permutations  $P$  form a group of  $N!$  elements, called the symmetric group [2]. Indeed,

- i) The *composition*  $R = QP$  of two permutations  $P$  and  $Q$  of the variables  $q_1, \dots, q_N$  is another permutation of the  $q_1, \dots, q_N$ .
- ii) The set of permutations  $P$  contains the *identity* permutation  $q_1 \rightarrow q_1, q_2 \rightarrow q_2, \dots, q_N \rightarrow q_N$ .
- iii) There exists a unique inverse  $P^{-1}$  of  $P$  which has the effect of sending  $q_{P1} \rightarrow q_1, q_{P2} \rightarrow q_2, \dots, q_{PN} \rightarrow q_N$ .

It is a simple matter to show that the permutations  $P$  are *linear* operators. If  $\psi$  and  $\chi$  are two wave functions depending on the variable set  $(q_1 \dots q_N)$ ,

$$P(a\psi + b\chi) = aP\psi + bP\chi \quad (7.6)$$

where  $a$  and  $b$  are constants. Moreover, the scalar product  $\langle \psi | \chi \rangle$  is left invariant by the permutation  $P$

$$\langle \psi | \chi \rangle = \langle P\psi | P\chi \rangle. \quad (7.7)$$

From this last property, and using the fact that  $P^{-1}$  is also a permutation, we see that

$$\langle \psi | P^\dagger \chi \rangle = \langle P\psi | \chi \rangle = \langle P^{-1}P\psi | P^{-1}\chi \rangle = \langle \psi | P^{-1}\chi \rangle \quad (7.8)$$

so that  $P^\dagger = P^{-1}$  and  $P$  is *unitary*.

We note that the  $N!$  permutations  $P$  do not all commute among themselves – except for the case  $N = 2$  – so that only a limited set of permutations can be diagonalized simultaneously with the Hamiltonian  $H$ . Therefore the eigenfunctions  $\psi_n(q_1, \dots, q_N)$  of  $H$  are not in general eigenfunctions of the permutation operators  $P$ . Thus, we write

$$P\psi_n = \sum_{n'} \langle n' | P | n \rangle \psi_{n'} \quad (7.9)$$

where  $\langle n' | P | n \rangle$  are matrix elements of  $P$  in the  $n$ -representation. They provide a matrix representation of the group, since the operation  $QP = R$  is easily seen to induce the matrix multiplication

$$\sum_{n''} \langle n' | Q | n'' \rangle \langle n'' | P | n \rangle = \langle n' | R | n \rangle. \quad (7.10)$$

Fortunately, we need not concern ourselves with the very rich structure of the symmetric group; it will be sufficient to consider *one-dimensional* representations of the group, such that

$$\langle n' | P | n \rangle = P_n \delta_{nn'}. \quad (7.11)$$

A first one-dimensional representation is obtained by simply choosing  $P_n = 1$  for all  $P$ . Then

$$P\psi_n(q_1, \dots, q_N) = \psi_n(q_{P1}, \dots, q_{PN}) = \psi_n(q_1, \dots, q_N). \quad (7.12)$$

In particular, for an interchange  $P_{ij}$ , we have

$$\begin{aligned} P_{ij}\psi_n(q_1, \dots, q_i, \dots, q_j, \dots, q_N) &= \psi_n(q_1, \dots, q_j, \dots, q_i, \dots, q_N) \\ &= \psi_n(q_1, \dots, q_i, \dots, q_j, \dots, q_N). \end{aligned} \quad (7.13)$$

Wave functions which satisfy eqs. (7.12)–(7.13) are said to be *symmetric*, and particles having states described by such symmetric wave functions are called *bosons*. They can be shown [e.g. 3] to obey Bose–Einstein statistics.

The second and last [4] one-dimensional representation of the symmetric group is obtained by choosing  $P_n = +1$  for an even permutation and  $P_n = -1$  for an odd permutation. Then

$$P\psi_n(q_1, \dots, q_N) = \psi_n(q_{P1}, \dots, q_{PN}) = \begin{cases} \psi_n(q_1, \dots, q_N) & \text{for an even permutation} \\ -\psi_n(q_1, \dots, q_N) & \text{for an odd permutation.} \end{cases} \quad (7.14)$$

In particular, for an interchange  $P_{ij}$ ,

$$\begin{aligned} P_{ij}\psi_n(q_1, \dots, q_i \dots q_j \dots q_N) &= \psi_n(q_1, \dots, q_j, \dots q_i \dots q_N) \\ &= -\psi_n(q_1, \dots, q_i \dots q_j, \dots q_N). \end{aligned} \quad (7.15)$$

Wave functions which satisfy eqs. (7.14)–(7.15) are said to be *antisymmetric*, and particles having states described by these wave functions are called *fermions*. They satisfy Fermi–Dirac statistics [e.g. 3].

Consider now individual (one-particle) states  $|q_\alpha\rangle_1, |q_\beta\rangle_2, \dots, |q_v\rangle_N$ , where the notation  $|q_\alpha\rangle_1$  means that particle 1 is in a state  $|q_\alpha\rangle$ , an eigenvector corresponding to the complete set of observables  $q_1$  and to the quantum number(s)  $\alpha$ . Symmetric and antisymmetric  $N$ -particle states  $|q_\alpha^{(1)}q_\beta^{(2)} \dots q_v^{(N)}\rangle_\pm$  may readily be constructed from these individual states [e.g. 5]. The antisymmetric state is given by the *Slater determinant*

$$|q_\alpha^{(1)}q_\beta^{(2)} \dots q_v^{(N)}\rangle_- = \frac{1}{\sqrt{N!}} \begin{vmatrix} |q_\alpha\rangle_1 & |q_\alpha\rangle_2 & \dots & |q_\alpha\rangle_N \\ |q_\beta\rangle_1 & |q_\beta\rangle_2 & \dots & |q_\beta\rangle_N \\ \vdots & \vdots & \ddots & \vdots \\ |q_v\rangle_1 & |q_v\rangle_2 & \dots & |q_v\rangle_N \end{vmatrix} \quad (7.16)$$

while the symmetric state  $|q_\alpha^{(1)}q_\beta^{(2)} \dots q_v^{(N)}\rangle_+$  is obtained from the same linear combination, but with all the signs being now positive. We note that antisymmetric states vanish when two or more of the individual quantum numbers are equal. This is precisely the content of the *Pauli (exclusion) principle* which is obeyed by fermions.

According to our present knowledge of particles occurring in nature, the two one-dimensional representations of the symmetric group, leading respectively to symmetric and antisymmetric wave functions are thought to be sufficient to describe all systems of identical particles. This is called the *symmetrization postulate* [6]. Experiment shows that spin  $\frac{1}{2}$  particles such as electrons, protons, neutrons, etc. . . . are fermions whereas integral spin particles such as the  $\pi$  and K mesons ( $s = 0$ ), the photon ( $s = 1$ ), etc. . . . are bosons. It is therefore strongly believed that a unique connection exists between the spin of a particle and the statistics that it obeys: half-integral spin particles are fermions, integral spin particles are bosons. A derivation of this connection from relativistic field theory was first proposed by Pauli [7].

We have just shown that a wave function must be properly symmetrized with respect to permutations of identical, “elementary” particles. We emphasize again that in the present discussion a particle should be considered as “elementary” if, in a given physical situation, we can ignore its possible composite structure. For example, in low-temperature physics, the properties of liquid  $^4\text{He}$  can be studied by treating the  $^4\text{He}$  atoms as “elementary” bosons. The symmetrization process is then accomplished with respect to

the permutation of the  ${}^4\text{He}$  atoms. On the other hand, if we wish to study the scattering of high-energy  ${}^4\text{He}$  nuclei on  ${}^4\text{He}$  nuclei, we must take into account the fact that the  ${}^4\text{He}$  nucleus contains two protons and two neutrons; the symmetrization of the wave function must then be performed with respect to the constituent protons and neutrons.

## 7.2. Boson-boson scattering

We now apply our discussion of the previous section to the scattering of two identical bosons of mass  $m$  in their center of mass coordinate system. For simplicity we shall consider only the case of spinless bosons.

Let us denote by  $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$  the position vector of the center of mass of the two particles, and by  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  their relative position vector. It is apparent that an interchange of the two identical particles does not affect the vector  $\mathbf{R}$  but changes the sign of  $\mathbf{r}$ .

The collision process between the two particles can be described by the symmetrized wave packet

$$Z_b(\mathbf{R}, \mathbf{r}, t) = u(\mathbf{R}, t) \frac{1}{\sqrt{2}} [\Psi_b(\mathbf{r}, t) + \Psi_b(-\mathbf{r}, t)] \quad (7.17)$$

where  $u(\mathbf{R}, t)$  is a normalized wave packet that keeps the position vector  $\mathbf{R}$  localized near  $\mathbf{R} = 0$  and  $\Psi_b(\mathbf{r}, t)$  is the wave packet discussed at length in Chapter 3. For  $t \rightarrow -\infty$ , we have

$$Z_b(\mathbf{R}, \mathbf{r}, t) \xrightarrow{t \rightarrow -\infty} Y_b(\mathbf{R}, \mathbf{r}, t) \quad (7.18a)$$

where

$$Y_b(\mathbf{R}, \mathbf{r}, t) = u(\mathbf{R}, t) \exp\{-i\mathbf{k}_i \cdot \mathbf{b} - \omega(k_i)t\} \\ \times \frac{1}{\sqrt{2}} [\exp(i\mathbf{k}_i \cdot \mathbf{r})\chi(\mathbf{r} - \mathbf{b} - \mathbf{v}_i t) + \exp(-i\mathbf{k}_i \cdot \mathbf{r})\chi(-\mathbf{r} - \mathbf{b} - \mathbf{v}_i t)] \quad (7.18b)$$

and the notation of Chapter 3 has been used [see eq. (3.87)]. We see from eq. (7.18b) that the wave packet  $Y_b(\mathbf{R}, \mathbf{r}, t)$  consists of two wave packets of norm  $\frac{1}{2}$ . The first one corresponds to the initial state of a collision in which particle 1 moves towards particle 2 with an average relative velocity  $\mathbf{v}_i = \hbar\mathbf{k}_i/\mu$  ( $\mu = \frac{1}{2}m$ ) and impact parameter  $\mathbf{b}$ . The second wave packet describes the same situation with particles 1 and 2 interchanged. Since the two wave packets do not overlap at  $t = -\infty$ , the symmetrized packet  $Y_b(\mathbf{R}, \mathbf{r}, t)$ , normalized to one, represents two particles moving towards each other in their center of mass frame with an average relative velocity  $\mathbf{v}_i$  and impact parameter  $\mathbf{b}$ .

For  $t \rightarrow +\infty$ , the symmetrized wave packet  $Z_b(\mathbf{R}, \mathbf{r}, t)$  becomes

$$Z_b(\mathbf{R}, \mathbf{r}, t) \xrightarrow{t \rightarrow +\infty} Y_b(\mathbf{R}, \mathbf{r}, t) + Z_b^{\text{sc}}(\mathbf{R}, \mathbf{r}, t) \quad (7.19a)$$

where the scattered part  $Z_b^{sc}(\mathbf{R}, \mathbf{r}, t)$  of the symmetrized wave packet is given by

$$Z_b^{sc}(\mathbf{R}, \mathbf{r}, t) = u(\mathbf{R}, t) \frac{1}{\sqrt{2}} [\Psi_b^{sc}(\mathbf{r}, t) + \Psi_b^{sc}(-\mathbf{r}, t)]. \quad (7.19b)$$

The corresponding symmetrized scattering amplitude then reads

$$f_+(\theta, \phi) = \frac{1}{\sqrt{2}} [f(\theta, \phi) + f(\pi - \theta, \phi + \pi)] \quad (7.20)$$

where we have used the fact that the polar coordinates of the vector  $-\mathbf{r}$  are given by  $(r, \pi - \theta, \phi + \pi)$ .

Let us now define the differential cross section as the number of particles emitted in the direction  $\Omega$  per unit time and per unit incident flux. Since the detection system cannot distinguish between particles 1 and 2, to each particle 1 emitted in the direction  $\Omega \equiv (\theta, \phi)$  there corresponds an identical particle 2 emitted in the opposite direction  $(\pi - \theta, \phi + \pi)$ . It is then natural to define

$$d\sigma/d\Omega = 2|f_+(\theta, \phi)|^2 = |f(\theta, \phi) + f(\pi - \theta, \phi + \pi)|^2. \quad (7.21)$$

It is important to note that with this definition of the differential cross section, the total cross section

$$\sigma_{\text{tot}} = \int |f(\theta, \phi) + f(\pi - \theta, \phi + \pi)|^2 d\Omega \quad (7.22)$$

is equal to twice the number of particles removed from the incident beam per unit time and unit incident flux.

We can also rewrite eq. (7.21) as

$$d\sigma/d\Omega = |f(\theta, \phi)|^2 + |f(\pi - \theta, \phi + \pi)|^2 + 2 \operatorname{Re} [f(\theta, \phi) f^*(\pi - \theta, \phi + \pi)]. \quad (7.23)$$

We note that in the classical limit, where the particles are distinguishable, the interference term [i.e. the third term on the right of eq. (7.23)] disappears. Hence the classical differential cross section

$$\frac{d\sigma_{cl}}{d\Omega} = |f(\theta, \phi)|^2 + |f(\pi - \theta, \phi + \pi)|^2 \quad (7.24)$$

is precisely the sum of the differential cross sections for observation of particle (1) in the direction  $(\theta, \phi)$  and of particle (2) in the opposite direction.

In the simple case where the amplitude  $f$  is independent of  $\phi$ , we deduce from eq. (7.21) that

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2 \quad (7.25)$$

so that the scattering is symmetric about  $\theta = \frac{1}{2}\pi$  in the center of mass system. We may also write eq. (7.25) as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |f(\pi - \theta)|^2 + 2\operatorname{Re}[f(\theta)f^*(\pi - \theta)]. \quad (7.26)$$

Since  $P_l[\cos(\pi - \theta)] = (-1)^l P_l(\cos \theta)$ , it is clear that the partial wave expansion of the symmetrized amplitude  $f_+(\theta)$  contains only *even* angular momenta. Moreover, at  $\theta = \frac{1}{2}\pi$ , we note that the quantum mechanical differential cross section (7.25) is *twice* as big as the classical result  $d\sigma_{cl}(\theta = \frac{1}{2}\pi)/d\Omega = 2|f(\theta = \frac{1}{2}\pi)|^2$ . Furthermore, if there is only s-wave ( $l = 0$ ) scattering, we see from eq. (7.25) that two colliding identical bosons exhibit a differential cross section four times as big as if they were considered as distinguishable, and twice as big as the classical result (7.24).

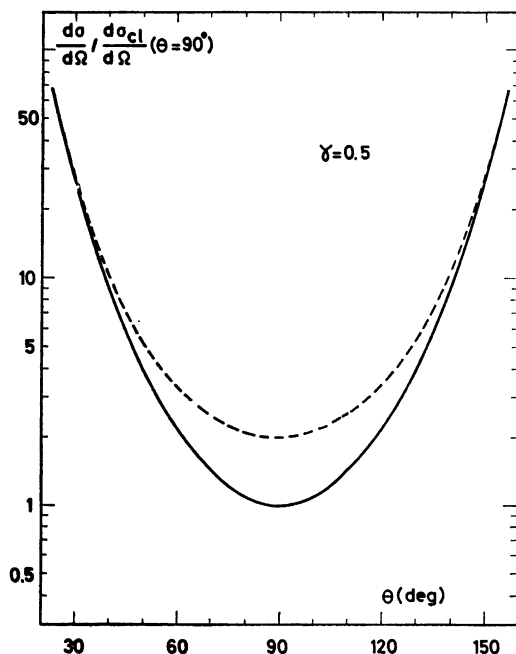


Fig. 7.1. The differential cross section  $d\sigma/d\Omega$  corresponding to the scattering of two identical bosons interacting through a Coulomb potential, divided by  $d\sigma_{cl}(\theta = 90^\circ)/d\Omega$ , for the value  $\gamma = (Ze)^2/\hbar v = 0.5$ . The dashed line represents the quantum mechanical result obtained by using the Mott formula (7.28) to calculate  $d\sigma/d\Omega$ . The solid curve shows the corresponding classical curve, obtained by omitting the last term on the right of eq. (7.28).

The non-classical effects due to the interference term in eq. (7.23) can also be illustrated for the case of Coulomb scattering. Let us consider two identical spinless bosons of charge  $Ze$  interacting only through Coulomb forces (as for example in low energy  ${}^4\text{He} - {}^4\text{He}$  scattering). Eq. (7.25) now reads

$$d\sigma/d\Omega = |f_c(\theta) + f_c(\pi - \theta)|^2 \quad (7.27)$$

where the Coulomb scattering amplitude  $f_c$  is given by eq. (6.32). Therefore [compare with the Rutherford formula (6.40)], we have

$$\frac{d\sigma}{d\Omega} = \left(\frac{\gamma}{2k}\right)^2 \left| \frac{\exp\{-2i\gamma \log(\sin \tfrac{1}{2}\theta)\}}{\sin^2 \tfrac{1}{2}\theta} + \frac{\exp\{-2i\gamma \log(\cos \tfrac{1}{2}\theta)\}}{\cos^2 \tfrac{1}{2}\theta} \right|^2$$

or

$$\begin{aligned} \frac{d\sigma}{d\Omega} = \left(\frac{\gamma}{2k}\right)^2 \{ & \text{cosec}^4 \tfrac{1}{2}\theta + \sec^4 \tfrac{1}{2}\theta \\ & + 2 \text{cosec}^2 \tfrac{1}{2}\theta \sec^2 \tfrac{1}{2}\theta \cos[2\gamma \log(\tan \tfrac{1}{2}\theta)] \} \end{aligned} \quad (7.28)$$

where  $\gamma = (Ze)^2/\hbar v$ , as given by eq. (6.10). The result (7.28) is called the *Mott formula* [8] for the Coulomb scattering of two identical spinless bosons.

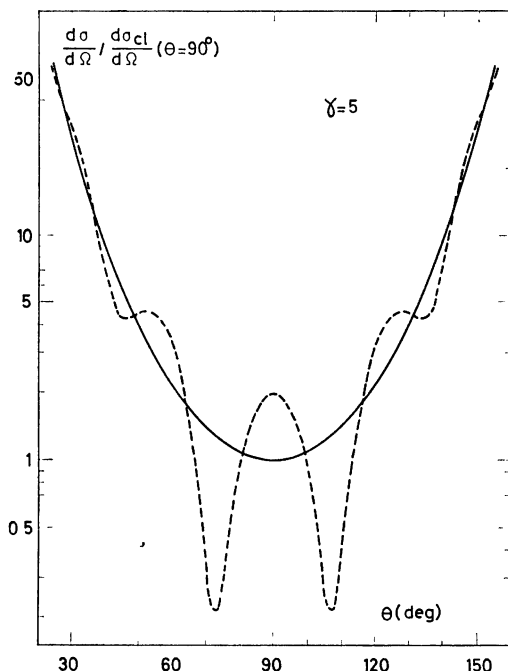


Fig. 7.2. Same as Fig. 7.1, but now  $\gamma = 5$ . Note the importance of the quantum-mechanical interference term around  $\theta = 90^\circ$ .

The corresponding classical calculation would only yield the first two terms on the right-hand side of eq. (7.28) [see eq. (7.24)]. We note that the interference term, which depends on  $\hbar$  through the quantity  $\gamma$ , oscillates increasingly about zero as  $\gamma$  becomes larger and (or) one departs from the angle  $\theta = \frac{1}{2}\pi$ . This is illustrated in Figs. 7.1 and 7.2, where the Mott and classical differential cross sections are shown when  $\gamma = 0.5$  and  $\gamma = 5$ , respectively. In the classical limit which is reached for  $\gamma \gg 1$ , the average value of the differential cross section (7.28) over a small solid angle  $\delta\Omega$  tends towards the classical cross section. We

note that the condition  $\gamma \gg 1$  corresponding to the classical limit is approached for *small* velocities. This is a peculiar feature of the Coulomb potential. We shall see in Chapter 9 that for potentials having a finite “range” the classical limit is approached for large  $v$ . We also verify that at  $\theta = \frac{1}{2}\pi$  the actual (quantum mechanical) differential cross section is twice as big as the classical one.

As an application of the foregoing discussion, let us consider the elastic scattering of two spinless  $^{12}\text{C}$  nuclei in their C.M. system. We shall assume that the C.M. kinetic energy  $K$  is low enough so that the effect of nuclear forces may be neglected and only the Coulomb interaction between the two  $^{12}\text{C}$  nuclei must be taken into account. For example, let us suppose that  $K = 5$  MeV, so that  $v \simeq 1.3 \times 10^9$  cm/sec and  $\gamma \simeq 6$ . We should therefore expect an angular distribution of the type given by the dashed curve of Fig. 7.2 (drawn for the nearby case  $\gamma = 5$ ). This is confirmed by experiment, as shown in Fig. 7.3. We see that the experimental points [9] are in excellent agreement with the Mott formula (7.28) and demonstrate very clearly the presence of the non-classical interference term.

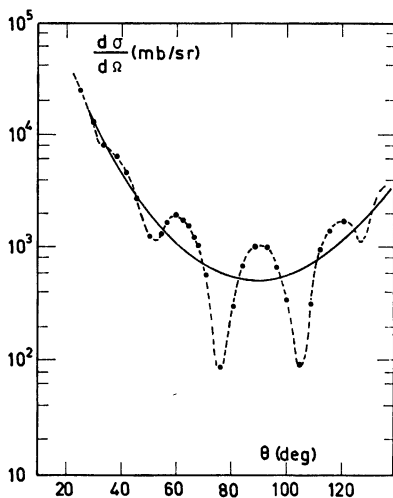


Fig. 7.3. The differential cross section corresponding to the elastic scattering of two  $^{12}\text{C}$  nuclei having a C.M. kinetic energy of 5 MeV. The dashed line represents the Mott formula (7.28). The solid curve shows the classical differential cross section. The dots are the experimental points of ref. [9].

### 7.3. Fermion–fermion scattering

The scattering of identical fermions is more difficult to treat than that of (spinless) bosons because of the complications arising from the spin. We shall confine ourselves here to the simple case of two spin  $\frac{1}{2}$  fermions whose



interaction is central. Since the interaction is in general different in the singlet ( $S = 0$ ) and triplet ( $S = 1$ ) spin states of the two fermions, we introduce two (unsymmetrized) amplitudes  $f_s(\theta)$  and  $f_t(\theta)$  corresponding respectively to the singlet and triplet cases.

The wave function describing this system of two identical spin  $\frac{1}{2}$  fermions must be antisymmetric in the interchange of the two fermions. Therefore, if the two spin  $\frac{1}{2}$  fermions are in a singlet spin state, the wave function is antisymmetric in the interchange of the spins and must therefore be symmetric in the interchange of the position vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$  of the two particles. Hence, the symmetrized singlet amplitude is

$$f_{s+}(\theta) = \frac{1}{\sqrt{2}}[f_s(\theta) + f_s(\pi - \theta)] \quad (7.29)$$

and the differential cross section in the singlet state is given by

$$(d\sigma/d\Omega)_s = 2|f_{s+}(\theta)|^2 = |f_s(\theta) + f_s(\pi - \theta)|^2. \quad (7.30)$$

If, on the contrary, the two spin  $\frac{1}{2}$  fermions are in a triplet spin state, the wave function is symmetric in the interchange of the spins and must therefore be antisymmetric in the interchange of the position vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . Thus the symmetrized triplet amplitude is given by

$$f_{t-}(\theta) = \frac{1}{\sqrt{2}}[f_t(\theta) - f_t(\pi - \theta)] \quad (7.31)$$

and the differential cross section in the triplet state reads

$$(d\sigma/d\Omega)_t = 2|f_{t-}(\theta)|^2 = |f_t(\theta) - f_t(\pi - \theta)|^2. \quad (7.32)$$

If the beam and target fermions are *unpolarized* (i.e. their spins are randomly oriented), the probability of generating triplet states is three times that of obtaining singlet states, so that the differential cross section becomes

$$\begin{aligned} d\sigma/d\Omega &= \frac{1}{4}(d\sigma/d\Omega)_s + \frac{3}{4}(d\sigma/d\Omega)_t \\ &= \frac{1}{4}|f_s(\theta) + f_s(\pi - \theta)|^2 + \frac{3}{4}|f_t(\theta) - f_t(\pi - \theta)|^2. \end{aligned} \quad (7.33)$$

For the case of spin-independent central interactions where

$$f_s(\theta) = f_t(\theta) = f(\theta) \quad (7.34)$$

we find from eq. (7.33) that [10]

$$d\sigma/d\Omega = |f(\theta)|^2 + |f(\pi - \theta)|^2 - \text{Re}[f(\theta)f^*(\pi - \theta)]. \quad (7.35)$$

Since the classical result [which corresponds to the neglect of the interference term in eq. (7.35)] is given by  $d\sigma_{cl}/d\Omega = |f(\theta)|^2 + |f(\pi - \theta)|^2$ , we note that at  $\theta = \frac{1}{2}\pi$  the quantum mechanical formula (7.35) yields *one-half* the classical answer  $d\sigma_{cl}(\theta = \frac{1}{2}\pi)/d\Omega$ . Furthermore, if there is only s-wave ( $l = 0$ ) scattering, the differential cross section (7.35) is four times smaller than the corresponding one [given by eq. (7.26)] for boson-boson scattering.

As an illustration of eq. (7.35) let us consider the case of Coulomb scattering of two identical spin  $\frac{1}{2}$  fermions of charge  $Ze$ . This could correspond for example to electron-electron (non-relativistic) scattering ( $Z = -1$ ) or proton-proton scattering ( $Z = +1$ ) at very low bombarding energies where the effect of nuclear forces can be neglected. Using the Coulomb amplitude  $f_c$  given by eq. (6.32), we obtain from eq. (7.35) the *Mott formula for the Coulomb scattering of two identical spin  $\frac{1}{2}$  fermions*, namely

$$\frac{d\sigma}{d\Omega} = \left(\frac{\gamma}{2k}\right)^2 \left\{ \text{cosec}^4 \frac{1}{2}\theta + \sec^4 \frac{1}{2}\theta - \text{cosec}^2 \frac{1}{2}\theta \sec^2 \frac{1}{2}\theta \cos[2\gamma \log(\tan \frac{1}{2}\theta)] \right\}. \quad (7.36)$$

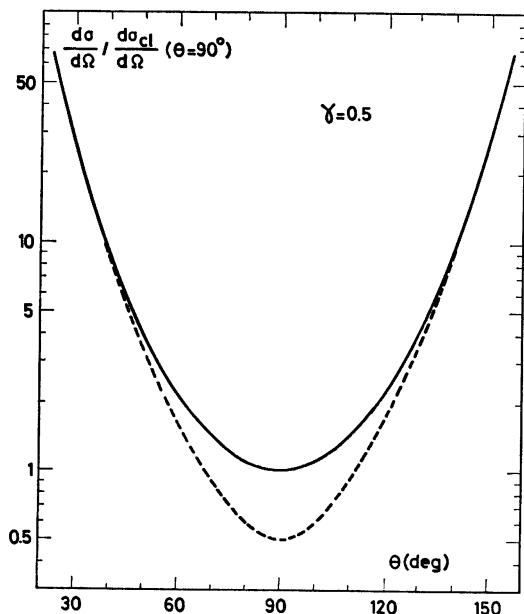


Fig. 7.4. The differential cross section  $d\sigma/d\Omega$  corresponding to the scattering of two identical fermions interacting through a Coulomb potential, divided by  $d\sigma_{cl}(\theta = 90^\circ)/d\Omega$  for the value  $\gamma = (Ze)^2/\hbar v = 0.5$ . The dashed curve represents the quantum mechanical result obtained by using the Mott formula (7.36) to calculate  $d\sigma/d\Omega$ . The solid curve shows the corresponding classical curve, obtained by omitting the last term on the right of eq. (7.36).

As in the case of eq. (7.28), the corresponding classical calculation would only yield the two first terms on the right-hand side of eq. (7.36). The effect of the interference term is shown in Figs. 7.4 and 7.5, where the Mott formula (7.36) and the classical calculation are shown for the cases  $\gamma = 0.5$  and  $\gamma = 5$ , respectively. Comparing Figs. 7.4 and 7.5 with the corresponding Figs. 7.1 and 7.2 for spinless identical boson-boson scattering, we see again

that the interference term oscillates more and more about zero as  $\gamma$  increases and (or) one leaves the scattering angle  $\theta = \frac{1}{2}\pi$ . In contrast with the boson-boson case, however, there is a *minimum* in the differential cross section for spin  $\frac{1}{2}$  identical fermion-fermion scattering at  $\theta = \frac{1}{2}\pi$ . At this value of the scattering angle the actual differential cross section is indeed smaller than the classical one by a factor of two, as we already pointed out above.

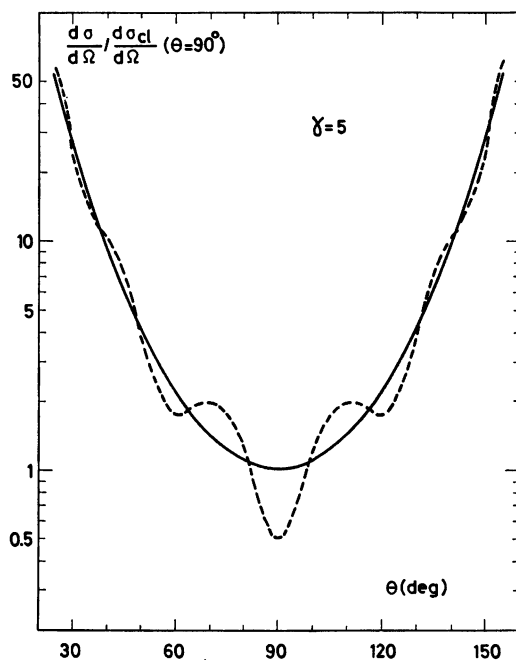


Fig. 7.5. Same as Fig. 7.4 but now  $\gamma = 5$ . Note the importance of the quantum mechanical interference term around  $\theta = 90^\circ$ .

## References and notes

- [1] We recall here our “definition” of Section 1.2: a particle is considered as “elementary” if in a given physical situation we can ignore its possible composite structure.
- [2] For a detailed study of the symmetric group, see for example WIGNER, E. P. (1959), *Group Theory* (Academic Press, New York) Chapter 13; HAMERMESH, M. (1964), *Group Theory* (Addison-Wesley, Reading, Mass.) Chapter 7.
- [3] MESSIAH, A. (1966), *Quantum Mechanics* (Wiley, New York) Vol. II, Chapter 14.
- [4] It can be shown that there exist only two one-dimensional representations of the symmetric group; see for example WIGNER, E. P., loc. cit. [2].
- [5] GOTTFRIED, K. (1966), *Quantum Mechanics. Volume I: Fundamentals* (Benjamin, New York) Section 41.

- [6] For  $N > 2$ , wave functions with more complicated permutation properties arise. They could correspond to hypothetical particles which would be neither bosons or fermions and obey modified (para) statistics. For a discussion of this point, see for example VOLKOV, D. V. (1959), *Zh. Eksp. i Teor. Fiz.* **36**, 1560 [*Soviet Phys. JETP* **9**, 1107]; MESSIAH, A. M. L. and O. W. GREENBERG (1964), *Phys. Rev.* **136**, B248; GREENBERG, O. W. and A. M. L. MESSIAH (1965), *Phys. Rev.* **138**, B1155; LANDSHOFF, P. V. and H. P. STAPP (1967), *Ann. Phys. (N.Y.)* **45**, 72.
- [7] PAULI, W. (1940), *Phys. Rev.* **58**, 716. A modern approach to this problem is given in STREATER, R. F. and A. S. WIGHTMAN (1964), *P.C.T., Spin and Statistics and All That* (Benjamin, New York).
- [8] MOTT, N. F. (1930), *Proc. Roy. Soc.* **A126**, 259.
- [9] BROMLEY, D. A., J. A. KUEHNER and E. ALMQVIST (1961), *Phys. Rev.* **123**, 878.
- [10] The generalization of the simple formula (7.35) and the corresponding equation (7.26) for spinless boson-boson scattering to any half integer or integer spin  $s$  may be carried out in a straightforward way. One finds

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |f(\pi - \theta)|^2 + \frac{(-1)^{2s}}{2s+1} 2 \operatorname{Re}[f(\theta)f^*(\pi - \theta)].$$

## The Born Series

We shall now begin our discussion of some approximation methods which are widely used in scattering theory. Approximate treatments are obviously necessary in complicated physical situations where exact solutions are not available. It is convenient, however, to consider them whenever possible [1] in the simple case of potential scattering, where their interpretation is simpler and their range of validity can be checked accurately.

We start in this chapter by studying the Born series, which is essentially a perturbation-type expansion of the wave function or the scattering amplitude in powers of the interaction potential. The basic idea and fundamental formulae of the method are given in Section 8.1. The first Born approximation is then studied in Section 8.2, while the higher terms of the Born series are discussed in Section 8.3. The next section deals with the problem of the convergence of the Born series. Section 8.5 is devoted to the Born series for partial waves. Finally, in Section 8.6 we illustrate the method by a detailed discussion of Yukawa-type potentials and of the separable non local interaction introduced in Section 5.7.

### *8.1. The Born expansion as a perturbation series*

Let us attempt to solve the Lippmann–Schwinger equation (5.33) by iteration, starting with the plane wave  $\Phi_{k_1}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_1 \cdot \mathbf{r})$  as the zero order approximation. We obtain in this way the sequence of functions

$$\begin{aligned}\psi_0(\mathbf{r}) &= \Phi_{k_1}(\mathbf{r}) \\ \psi_1(\mathbf{r}) &= \Phi_{k_1}(\mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \Phi_{k_1}(\mathbf{r}') d\mathbf{r}'\end{aligned}$$

$$\begin{aligned}
\psi_2(\mathbf{r}) &= \Phi_{k_1}(\mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_1(\mathbf{r}') d\mathbf{r}' \\
&\vdots \\
\psi_n(\mathbf{r}) &= \Phi_{k_1}(\mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_{n-1}(\mathbf{r}') d\mathbf{r}'
\end{aligned} \tag{8.1}$$

where the Green's function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  is given by eq. (5.27) and we have assumed that the interaction potential is real and local. We may also write the function  $\psi_n$  in the form

$$\psi_n(\mathbf{r}) = \sum_{m=0}^n \phi_m(\mathbf{r}), \tag{8.2}$$

where

$$\phi_0(\mathbf{r}) = \psi_0(\mathbf{r}) = \Phi_{k_1}(\mathbf{r}), \tag{8.3}$$

$$\phi_1(\mathbf{r}) = \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \Phi_{k_1}(\mathbf{r}') d\mathbf{r}' = \int K_1(\mathbf{r}, \mathbf{r}') \Phi_{k_1}(\mathbf{r}') d\mathbf{r}' \tag{8.4}$$

with

$$K_1(\mathbf{r}, \mathbf{r}') = G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \tag{8.5}$$

and

$$\phi_m(\mathbf{r}) = \int K_m(\mathbf{r}, \mathbf{r}') \Phi_{k_1}(\mathbf{r}') d\mathbf{r}', \quad m \geq 2 \tag{8.6}$$

with

$$K_m(\mathbf{r}, \mathbf{r}') = \int K_1(\mathbf{r}, \mathbf{r}'') K_{m-1}(\mathbf{r}'', \mathbf{r}') d\mathbf{r}'', \quad m \geq 2. \tag{8.7}$$

The Born series for the scattering wave function is obtained by letting  $n \rightarrow \infty$  in eq. (8.2). We see from eqs. (8.3)–(8.7) that it is a *perturbation series in powers of the potential*. Assuming that the sequence (8.1) converges towards the exact solution  $\psi_{k_1}^{(+)}$  of the scattering problem, we may then write eq. (8.2) as

$$\psi_{k_1}^{(+)}(\mathbf{r}) = \sum_{m=0}^{\infty} \phi_m(\mathbf{r}). \tag{8.8}$$

Let us now consider the integral representation (5.40) of the scattering amplitude. If we replace in it the exact scattering wave function  $\psi_{k_1}^{(+)}$  successively by the functions of the sequence (8.1) we obtain the corresponding sequence

$$f_{B1} = -2\pi^2 \langle \Phi_{k_t} | U | \Phi_{k_1} \rangle \tag{8.9}$$

$$f_{B2} = -2\pi^2 \langle \Phi_{k_t} | U | \psi_1 \rangle \tag{8.10}$$

$\vdots$

$$f_{Bn} = -2\pi^2 \langle \Phi_{k_t} | U | \psi_{n-1} \rangle. \tag{8.11}$$

The quantities  $f_{B1}, f_{B2}, \dots, f_{Bn}$  are called respectively the first Born approximation, the second Born approximation,  $\dots$   $n$ th Born approximation to the scattering amplitude. Using eq. (8.2) and setting  $j = m + 1$  we may also write eq. (8.11) as

$$f_{Bn} = \sum_{j=1}^n \bar{f}_{Bj} \quad (8.12)$$

where the expression  $\bar{f}_{Bj}$  is given by

$$\bar{f}_{Bj} = -2\pi^2 \langle \Phi_{k_t} | U | \phi_{j-1} \rangle, \quad j \geq 1 \quad (8.13)$$

or, using eqs. (8.3)–(8.7)

$$\bar{f}_{Bj} = -2\pi^2 \langle \Phi_{k_t} | U G_0^{(+)} U \dots G_0^{(+)} U | \Phi_{k_i} \rangle. \quad (8.14)$$

We see that the quantity  $\bar{f}_{Bj}$  contains  $j$  times the potential and  $(j - 1)$  times the free Green's function  $G_0^{(+)}$ . We shall call it the *term of order  $j$*  in the sum (8.12). For example

$$\bar{f}_{B1} = f_{B1} = -2\pi^2 \langle \Phi_{k_t} | U | \Phi_{k_i} \rangle \quad (8.15)$$

and

$$\bar{f}_{B2} = -2\pi^2 \langle \Phi_{k_t} | U G_0^{(+)} U | \Phi_{k_i} \rangle \quad (8.16)$$

so that

$$f_{B2} = f_{B1} + \bar{f}_{B2}. \quad (8.17)$$

The *Born series for the scattering amplitude* is defined by letting  $n \rightarrow \infty$  in eq. (8.12). If this series converges towards the exact scattering amplitude  $f$ , one may write

$$f = \sum_{j=1}^{\infty} \bar{f}_{Bj}. \quad (8.18)$$

It is worth noting that the successive Born approximations  $f_{B1}, f_{B2}, \dots, f_{Bn}$  to the scattering amplitude may also be obtained by considering the asymptotic behaviour of the functions  $\psi_1, \psi_2, \dots, \psi_n$  belonging to the sequence (8.1) and following the arguments leading to eq. (5.40). For example, we have

$$\psi_1(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) + f_{B1} \frac{\exp(ikr)}{r} \right] \quad (8.19)$$

where  $f_{B1}$  is given by eq. (8.9)

A Born series similar to that of the scattering amplitude may evidently also be defined for the *transition matrix element*  $T_{fi}$  given by eq. (5.43). Thus we have

$$T_{fi} = \sum_{j=1}^{\infty} \bar{T}_{fi}^{Bj} \quad (8.20)$$

where

$$\bar{T}_{fi}^{B1} = T_{fi}^{B1} = \langle \Phi_{k_t} | V | \Phi_{k_i} \rangle \quad (8.21)$$

and

$$T_{fi}^{Bj} = \langle \Phi_{k_f} | V G_0^{(+)} V \cdots G_0^{(+)} V | \Phi_{k_i} \rangle. \quad (8.22)$$

In this last expression the potential  $V$  appears  $j$  times while the free Green's function

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') = -\frac{m}{2\pi\hbar^2} \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \quad (8.23)$$

appears  $(j - 1)$  times. The  $n$ th Born approximation to the transition matrix element is then given by

$$T_{fi}^{Bn} = \sum_{j=1}^n T_{fi}^{Bj}. \quad (8.24)$$

Another way of generating the Born series is to solve the integral equation (5.52) for the total Green's function by successive iterations, starting from  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  as the zero-order approximation. In this way, we generate the development

$$\begin{aligned} G^{(+)}(\mathbf{r}, \mathbf{r}') &= G_0^{(+)}(\mathbf{r}, \mathbf{r}') + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}_1) U(\mathbf{r}_1) G_0^{(+)}(\mathbf{r}_1, \mathbf{r}') d\mathbf{r}_1 \\ &+ \int G_0^{(+)}(\mathbf{r}, \mathbf{r}_1) U(\mathbf{r}_1) G_0^{(+)}(\mathbf{r}_1, \mathbf{r}_2) U(\mathbf{r}_2) G_0^{(+)}(\mathbf{r}_2, \mathbf{r}') d\mathbf{r}_1 d\mathbf{r}_2 + \cdots \end{aligned} \quad (8.25)$$

which defines the Born series for the total Green's function  $G^{(+)}(\mathbf{r}, \mathbf{r}')$ . Retaining in this expansion the terms up to order  $(n - 1)$  in the potential and substituting in the formal solution (5.50), we recover the  $n$ th Born approximation for  $\psi_{k_i}^{(+)}(\mathbf{r})$ , namely  $\psi_n(\mathbf{r})$ .

## 8.2. The first Born approximation [2]

We shall now analyze more closely the first Born approximation (8.9). Because  $\Phi_{k_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r})$  and  $\Phi_{k_f}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r})$ , we find that the matrix element (8.9), evaluated in the coordinate representation, is given by

$$f_{B1} = -2\pi^2 \langle \Phi_{k_f} | U | \Phi_{k_i} \rangle = -\frac{1}{4\pi} \int \exp\{i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}\} U(\mathbf{r}) d\mathbf{r}. \quad (8.26)$$

Let us introduce the wave vector transfer (see Fig. 8.1)

$$\Delta = \mathbf{k}_i - \mathbf{k}_f \quad (8.27)$$

so that

$$\hbar\Delta = \hbar(\mathbf{k}_i - \mathbf{k}_f) = \mathbf{p}_i - \mathbf{p}_f \quad (8.28)$$

is the momentum transfer which occurs during the collision. We note that since we are considering the scattering by a real potential, only elastic



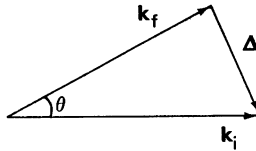


Fig. 8.1. The initial wave vector  $k_i$ , final wave vector  $k_f$ , and wave vector transfer  $\Delta$ . For elastic scattering one has  $k = |k_i| = |k_f|$  and the magnitude of the momentum transfer is  $2\hbar k \sin \frac{1}{2}\theta$ .

scattering is allowed and we have  $|k_i| = |k_f| = k$ . Hence the magnitude of the vector  $\Delta$  is given from eq. (8.27) by [3]

$$\Delta = 2k \sin \frac{1}{2}\theta \quad (8.29)$$

where  $\theta$  is the scattering angle, as shown on Fig. 8.1. Returning to eq. (8.26), we see that

$$f_{B1}(k, \theta, \phi) = -\frac{1}{4\pi} \int \exp(i\Delta \cdot \mathbf{r}) U(\mathbf{r}) \, d\mathbf{r} \quad (8.30)$$

so that the first Born scattering amplitude for a given direction  $(\theta, \phi)$  is proportional to the *Fourier transform of the potential* corresponding to the wave vector transferred during the collision.

The differential cross section in the first Born approximation is evidently given by

$$(d\sigma/d\Omega)_{B1} = |f_{B1}|^2. \quad (8.31)$$

We see that it is unchanged when  $U(\mathbf{r})$  is replaced by  $-U(\mathbf{r})$ . The total first Born cross section is simply

$$\sigma_{\text{tot}}^{B1}(k) = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta |f_{B1}(k, \theta, \phi)|^2. \quad (8.32)$$

For a *central* potential  $U(r)$ , the angular integrals in eq. (8.30) are readily performed by choosing the vector  $\Delta$  as the polar axis. Then

$$f_{B1}(k, \theta) = -\frac{1}{\Delta(k, \theta)} \int_0^\infty r \sin \{\Delta(k, \theta)r\} U(r) \, dr \quad (8.33)$$

where  $\Delta$  is given by eq. (8.29). We verify that the scattering amplitude (8.33) is independent of the azimuthal angle  $\phi$ , as it always should be for a central potential. We also note that  $f_{B1}$ , as given by eq. (8.33) is *real*. Moreover, it depends on the scattering angle  $\theta$  and the wave number  $k$  only through the quantity  $\Delta$ . The total Born cross section is now given by

$$\sigma_{\text{tot}}^{B1}(k) = 2\pi \int_0^\pi d\theta \sin \theta |f_{B1}(k, \theta)|^2. \quad (8.34)$$

In performing this integral it is convenient to take advantage of the fact that  $f_{B1}$  only depends on  $\Delta$  for a central potential. For the sake of simplicity, we

shall avoid the introduction of a new symbol and write  $f_{B1}(k, \theta) \equiv f_{B1}(\Delta)$ , with

$$f_{B1}(\Delta) = -\frac{1}{\Delta} \int_0^\infty r \sin(\Delta r) U(r) dr. \quad (8.35)$$

Then, choosing  $\Delta$  as the new variable of integration in eq. (8.34) and using eq. (8.29), we find that  $\sin \theta d\theta = \Delta d\Delta/k^2$  and therefore

$$\sigma_{\text{tot}}^{B1}(k) = \frac{2\pi}{k^2} \int_0^{2k} |f_{B1}(\Delta)|^2 \Delta d\Delta. \quad (8.36)$$

At high incident energies ( $k \rightarrow \infty$ ) we may obtain the asymptotic form of eq. (8.36) by writing

$$\sigma_{\text{tot}}^{B1}(k) \underset{k \rightarrow \infty}{\sim} \frac{2\pi}{k^2} \int_0^\infty |f_{B1}(\Delta)|^2 \Delta d\Delta \quad (8.37)$$

so that the quantity  $\sigma_{\text{tot}}^{B1}$  tends to zero as  $k^{-2}$ , i.e. as the inverse of the energy  $E = \hbar^2 k^2 / 2m$ .

### 8.3. The Born series

Let us now examine the higher terms of the Born series for the scattering amplitude. The *second* Born approximation  $f_{B2}$  is given by eq. (8.17) where the quantity  $\tilde{f}_{B2}$ , the true second order part of  $f_{B2}$  is defined by the matrix element (8.16). If we continue to use the coordinate representation, we see that  $\tilde{f}_{B2}$  may be written more explicitly as

$$\tilde{f}_{B2} = -\frac{1}{4\pi} \int d\mathbf{r} d\mathbf{r}' \exp(-i\mathbf{k}_f \cdot \mathbf{r}) U(\mathbf{r}) G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \exp(i\mathbf{k}_i \cdot \mathbf{r}'). \quad (8.38)$$

More generally, the  $n$ th Born approximation  $f_{Bn}$  to the scattering amplitude is obtained from eq. (8.12), where the quantity  $\tilde{f}_{Bj}$ , given by eq. (8.14), may be written by using the coordinate representation as

$$\begin{aligned} \tilde{f}_{Bj} = -\frac{1}{4\pi} \int d\mathbf{r}_1 \dots d\mathbf{r}_j \exp(-i\mathbf{k}_f \cdot \mathbf{r}_1) U(\mathbf{r}_1) G_0^{(+)}(\mathbf{r}_1, \mathbf{r}_2) U(\mathbf{r}_2) \dots \\ G_0^{(+)}(\mathbf{r}_{j-1}, \mathbf{r}_j) U(\mathbf{r}_j) \exp(i\mathbf{k}_i \cdot \mathbf{r}_j). \end{aligned} \quad (8.39)$$

It is also useful to analyze the expression of  $\tilde{f}_{Bj}$  [eq. (8.14)] in *momentum space*. Defining

$$\langle \mathbf{q} | U | \mathbf{q}' \rangle = (2\pi)^{-3} \int \exp\{i(\mathbf{q}' - \mathbf{q}) \cdot \mathbf{r}\} U(\mathbf{r}) d\mathbf{r} \quad (8.40)$$

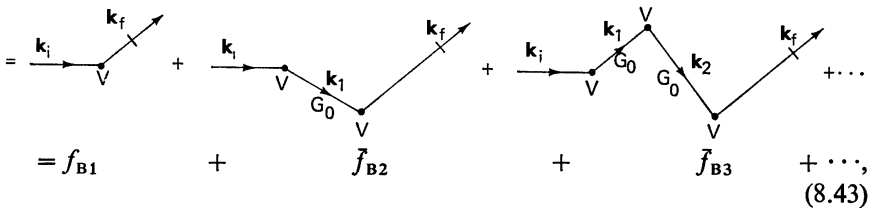
and using the integral representation (5.30) of the Green's function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$ , we find that

$$f_{B1} = \tilde{f}_{B1} = -2\pi^2 \langle \Phi_{\mathbf{k}_f} | U | \Phi_{\mathbf{k}_i} \rangle = -2\pi^2 \langle \mathbf{k}_f | U | \mathbf{k}_i \rangle \quad (8.41)$$

and

$$\begin{aligned} \tilde{f}_{Bj} = & -2\pi^2 \int dk_1 dk_2 \dots dk_{j-1} \langle k_f | U | k_{j-1} \rangle \frac{1}{k^2 - k_{j-1}^2 + i\epsilon} \langle k_{j-1} | U | k_{j-2} \rangle \\ & \times \frac{1}{k^2 - k_{j-2}^2 + i\epsilon} \langle k_{j-2} | U | k_{j-3} \rangle \dots \\ & \langle k_2 | U | k_1 \rangle \frac{1}{k^2 - k_1^2 + i\epsilon} \langle k_1 | U | k_i \rangle. \end{aligned} \quad (8.42)$$

The formulae (8.39) and (8.42) justify the interpretation of the Green's function as a *propagator*, while the quantities  $k_1, k_2, \dots, k_{j-1}$  are called "intermediate momenta". We can therefore visualize the Born series by writing the scattering amplitude as



$$= \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \dots$$

$$= f_{B1} + \tilde{f}_{B2} + \tilde{f}_{B3} + \dots, \quad (8.43)$$

i.e. as a *multiple scattering series* in which the projectile interacts repeatedly with the potential and propagates freely between two such interactions. Looking at the diagrams of eq. (8.43) we expect that the Born series will converge (i.e. that the higher order terms will be negligible compared to the first few terms) if the incident particle is sufficiently "fast" so that it cannot interact many times with the potential and/or if the potential is "weak" enough. These intuitive considerations in fact yield the correct conditions for the convergence of the Born series, as we shall see below.

It is interesting to analyze the relationship between the optical theorem (3.55) and the Born series. Let us write the scattering amplitude as

$$f = \lambda f_{B1} + \lambda^2 \tilde{f}_{B2} + \lambda^3 \tilde{f}_{B3} + \dots \quad (8.44)$$

where we have displayed explicitly the order of the perturbation expansion in terms of a parameter  $\lambda$ . Then, using eq. (3.55) and equating the coefficients of equal powers of  $\lambda$  we find that

$$\begin{aligned} \text{Im } f_{B1}(\theta = 0) &= 0 \\ \int d\Omega |f_{B1}|^2 &= \frac{4\pi}{k} \text{Im } \tilde{f}_{B2}(\theta = 0) \\ \int d\Omega [f_{B1} \tilde{f}_{B2}^* + f_{B1}^* \tilde{f}_{B2}] &= \frac{4\pi}{k} \text{Im } \tilde{f}_{B3}(\theta = 0), \\ \int d\Omega [f_{B1} \tilde{f}_{B3}^* + f_{B1}^* \tilde{f}_{B3} + |\tilde{f}_{B2}|^2] &= \frac{4\pi}{k} \text{Im } \tilde{f}_{B4}(\theta = 0), \text{ etc. } \dots \end{aligned} \quad (8.45)$$

These relations simplify for a central potential, in which case  $f_{B1} = f_{B1}^*$  as we have seen above. The first of eqs. (8.45) simply shows that the first Born scattering amplitude does not satisfy the optical theorem (or “violates unitarity”). The second equation which we can rewrite as

$$\sigma_{\text{tot}}^{B1} = \frac{4\pi}{k} \text{Im } \tilde{f}_{B2}(\theta = 0) = \frac{4\pi}{k} \text{Im } f_{B2}(\theta = 0) \quad (8.46)$$

illustrates the *non-linear* character of the optical theorem. Indeed, it relates the total first Born cross section  $\sigma_{\text{tot}}^{B1}$  (obtained by integrating the differential cross section  $|f_{B1}|^2$  over the angles) to the imaginary part of the forward second Born amplitude. This equation provides a useful check in performing second Born calculations. A similar, but more general analysis than the above one may be made by starting from the unitarity relation (4.94) instead of the optical theorem.

#### 8.4. Convergence of the Born series [4–9]

To study the convergence of the Born series, we start from the following theorem [e.g. 10]:

“If  $K(x, y) \in \mathcal{L}^2$  and  $g(x) \in \mathcal{L}^2$ , the integral equation

$$f(x) = g(x) + \lambda \int_a^b K(x, y)f(y) dy \quad (8.47)$$

has one and only one solution  $\in \mathcal{L}^2$ , given by the Liouville–Neumann series

$$f(x) = g(x) + \lambda g_1(x) + \lambda^2 g_2(x) + \dots \quad (8.48)$$

where

$$g_n(x) = \int K^n(x, y)g(y) dy \quad (8.49)$$

provided that [11]

$$|\lambda| \left[ \int_a^b dx \int_a^b dy |K(x, y)|^2 \right]^{1/2} < 1. \quad (8.50)$$

The series (8.48) then converges absolutely and uniformly in  $x$  in the interval  $(a, b)$ .”

The above theorem, which is readily generalized to an arbitrary number of dimensions, is not directly applicable to the Lippmann–Schwinger equation (5.33) since the kernel of this equation and the function  $\Phi_{k_i}(\mathbf{r})$  are not square integrable. To remedy this difficulty, we may use again the methods of Chapter 5. For example, using eqs. (5.119)–(5.121), we rewrite the Lippmann–Schwinger equation (5.33) as

$$\tilde{\psi}_{k_i}^{(+)}(\mathbf{r}) = \tilde{\Phi}_{k_i}(\mathbf{r}) + \int \tilde{K}(\mathbf{r}, \mathbf{r}') \tilde{\psi}_{k_i}^{(+)}(\mathbf{r}') d\mathbf{r}'. \quad (8.51)$$

The Born series, which coincides with the Liouville–Neumann series for eq. (8.51) will therefore converge if

$$\left[ \int d\mathbf{r} d\mathbf{r}' |\tilde{K}(\mathbf{r}, \mathbf{r}')|^2 \right]^{1/2} < 1 \quad (8.52)$$

or, for real  $k$ ,

$$\frac{1}{4\pi} \left[ \int d\mathbf{r} d\mathbf{r}' |U(\mathbf{r})| |U(\mathbf{r}')| \frac{1}{|\mathbf{r} - \mathbf{r}'|^2} \right]^{1/2} < 1. \quad (8.53)$$

Defining the quantity

$$B = \frac{1}{4\pi} \max_{(\mathbf{r})} \int |U(\mathbf{r}')| d\mathbf{r}' \quad (8.54)$$

where the notation  $\max_{(\mathbf{r})}$  means that we are taking the maximum by varying  $\mathbf{r}$ , we see that a *sufficient condition* for convergence of the Born series at all energies is given by [6]

$$B < 1. \quad (8.55)$$

In the particular case of a central potential satisfying the requirements (5.134)–(5.135), this condition reduces to

$$\int_0^\infty r |U(r)| dr < 1. \quad (8.56)$$

Since Bargmann [12] has shown that the number  $n_{b,l}$  of bound states of angular momentum  $l$  in a central potential  $-|U(r)|$  is such that

$$(2l + 1)n_{b,l} < \int_0^\infty r |U(r)| dr \quad (8.57)$$

we conclude that, *for a central potential  $U(r)$  satisfying the conditions (5.134)–(5.135), the Born series converges for all energies if the potential  $-|U(r)|$  does not support any bound state.*

Another important result, proved by Zemach and Klein [6], is that *the Born series converges at sufficiently high energies* [13], for central potentials  $U(r)$  less singular than  $r^{-2}$  at  $r = 0$  and decreasing to zero faster than  $r^{-3}$  as  $r \rightarrow \infty$ . These two conclusions confirm and state more precisely the intuitive arguments about the convergence of the Born series developed after eq. (8.43).

To conclude this section, let us give a simple nonrigorous way of deriving sufficient conditions for the validity of the first Born approximation. Let us write the exact scattering wave function  $\psi_{\mathbf{k}_1}^{(+)}(\mathbf{r})$  as

$$\psi_{\mathbf{k}_1}^{(+)}(\mathbf{r}) = \Phi_{\mathbf{k}_1}(\mathbf{r}) + \psi_{\text{sc}}^{+}(\mathbf{r}). \quad (8.58)$$

Assuming that  $|\psi_{\text{sc}}^{+}(\mathbf{r})|$  reaches its maximum value at the “center”  $\mathbf{r} = 0$  of the potential, we require in order for our perturbation approach to be valid that

$$|\psi_{\text{sc}}^{+}(0)| \ll |\Phi_{\mathbf{k}_1}(\mathbf{r})| = (2\pi)^{-3/2}. \quad (8.59)$$

To obtain an estimate of  $\psi_{sc}^{(+)}(\mathbf{r})$ , let us return to eq. (8.1) and assume that the exact scattering wave function  $\psi_{k_i}^{(+)}(\mathbf{r})$  may be approximated by the function  $\psi_1(\mathbf{r})$ . Then

$$\psi_{sc}^{(+)}(\mathbf{r}) \simeq -\frac{1}{4\pi} \int \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') d\mathbf{r}' \quad (8.60)$$

so that eq. (8.59) may be written as

$$\frac{1}{4\pi} \left| \int \frac{\exp(ikr')}{r'} U(\mathbf{r}') \exp(ik_i \cdot \mathbf{r}') d\mathbf{r}' \right| \ll 1. \quad (8.61)$$

For a central potential of “strength”  $|U_0|$  and “range”  $a$  (square well or square barrier) the angular integrations are easily performed. We find

$$\frac{|U_0|}{4k^2} |e^{2ika} - 2ika - 1| \ll 1. \quad (8.62)$$

For low energies ( $ka \rightarrow 0$ ) this condition becomes

$$\frac{1}{2}|U_0|a^2 \ll 1. \quad (8.63)$$

Remembering that a square well binds a particle when

$$\frac{1}{2}|U_0|a^2 > \frac{1}{8}\pi^2 \simeq 1 \quad (8.64)$$

we verify that the first Born approximation is valid at low energies only if the potential is very “weak”.

At high energies, the condition (8.62) yields

$$|V_0|a/\hbar v = |U_0|a/2k \ll 1 \quad (8.65)$$

where  $V_0 = (\hbar^2/2m)U_0$  and  $v$  is the magnitude of the particle velocity. Hence the first Born approximation is correct for sufficiently large incoming energies, as stated above. How large must the incident energy be depends evidently on the particular problem considered. We note that the quantity  $\tau_1 = a/v$  represents roughly the time spent by the particle in the range of the potential, while  $\tau_2 = \hbar/|V_0|$  corresponds to a time necessary for the potential to have a significant effect. The condition (8.65) therefore shows that the first Born approximation is valid if the ratio  $\tau_1/\tau_2$  is small, as we expect on physical grounds.

Let us illustrate these simple criteria with a few examples. Consider first the elastic scattering of an electron by a neutral atom. We shall describe approximately the electron-atom interaction by the screened Coulomb or Yukawa potential [14]

$$V(r) = -\frac{Ze^2}{r} e^{-r/a} \quad (8.66)$$

where  $Z$  is the atomic number of the target and where the length  $a$ , which measures the linear dimension of the atomic electron cloud can be estimated from the Thomas-Fermi model of the atom; it is given by

$$a \simeq a_0/Z^{1/3} \quad (8.67)$$

$a_0 = \hbar^2/me^2$  being the "first Bohr radius". The criterion (8.61) then becomes

$$\frac{2Z}{ka_0} \left| \int_0^\infty \exp\left\{ix - \frac{x}{ka}\right\} \frac{\sin x}{x} dx \right| \ll 1 \quad (8.68)$$

where  $x = kr'$  is the new variable of integration. For low energies ( $ka \ll 1$ ) we obtain, using eq. (8.67)

$$2Za/a_0 = 2Z^{2/3} \ll 1 \quad (8.69)$$

which shows that the Born approximation cannot be used in this case. For high energies ( $ka \gg 1$ ), eq. (8.68) yields

$$(Ze^2/\hbar v) \log ka \ll 1 \quad (8.70)$$

a result comparable to eq. (8.65) with  $|V_0| \simeq Ze^2/a$ . Thus for incident velocities large compared to atomic velocities [15] we expect the Born approximation to be valid in this case.

As a second example, let us consider nucleon-nucleon scattering described by the Yukawa potential

$$V(r) = -V_0 e^{-\mu r}/\mu r. \quad (8.71)$$

For the choice  $V_0 \simeq 50$  MeV and  $\mu = a^{-1} \simeq 0.7 \times 10^{13} \text{ cm}^{-1}$  corresponding to the neutron-proton interaction in the state  ${}^3S_1$ , we find that the criterion (8.65) is only satisfied if the (C.M.) energy is several hundreds of MeV. Since in that case the description of nucleon-nucleon scattering by a potential is not justified we do not expect the Born approximation to be very useful in this problem.

### 8.5. The Born series for partial waves

The Born development provides an expansion for the total scattering amplitude  $f(k, \theta, \phi)$ , but it can equally well be applied to the analysis in partial waves. With the "normalization"

$$R_l(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) - \tan \delta_l n_l(kr) \quad (8.72)$$

the (one-dimensional) radial integral equations for the radial wave functions  $R_l(k, r)$  read [see eqs. (5.98)–(5.99)]

$$R_l(k, r) = j_l(kr) + \int_0^\infty G_l(r, r') U(r') R_l(k, r') r'^2 dr'. \quad (8.73)$$

Let us solve these equations by successive iterations. Starting from the zero-order approximation  $R_l^{(0)}(k, r) = j_l(kr)$ , we obtain at once from eq. (5.96) the *first Born approximation* for the tangent of the phase shift, namely

$$(\tan \delta_l)_{B1} = -k \int_0^\infty [j_l(kr)]^2 U(r) r^2 dr. \quad (8.74)$$

The *second Born approximation* for  $\tan \delta_l$  is obtained by iterating once eq. (8.73) [using  $R_l^{(0)}$  as input on the right-hand side] and substituting the resulting radial function in eq. (5.96). This yields

$$(\tan \delta_l)_{B2} = -k \left\{ \int_0^\infty [j_l(kr)]^2 U(r) r^2 dr + \int_0^\infty dr \int_0^\infty dr' j_l(kr) U(r) G_l(r, r') U(r') j_l(kr') r^2 r'^2 \right\}. \quad (8.75)$$

Higher Born approximations for  $\tan \delta_l$  are obtained by a straightforward generalization of this reasoning.

Kohn [5] has made a detailed investigation of the convergence of the Born series as applied to the partial wave analysis. He finds that, for zero-energy scattering ( $k = 0$ ) the Born series converges if

$$\int_0^\infty r |U(r)| dr < 2l + 1 \quad (8.76)$$

which, using Bargmann's condition (8.57), shows that the potential  $-|U(r)|$  cannot support a bound state of angular momentum  $l$ .

At high energies, and for a "regular" potential such that

$$\int_0^1 |U(r)| dr < \infty \quad (8.77)$$

the Born series converges if

$$\left| \int_0^\infty U(r) dr \right| < \pi k. \quad (8.78)$$

If the potential  $U(r)$  has an  $r^{-1}$  singularity at  $r = 0$ , we may write it as

$$U(r) = U_0 a F(r)/r \quad (8.79)$$

where  $F(r)$  is a dimensionless function of  $r$  such that  $F(0) = 1$  and we assume that the potential has a "range"  $a$ . Then a sufficient condition for the convergence of the Born series at high energies is that [5]

$$(|U_0|a/k)[\log(ka)/\pi] < 1. \quad (8.80)$$

It is often said that the Born approximation is good when the phase shifts are "small". This statement is not always correct, as can be illustrated in the case of the repulsive hard sphere potential. For the  $l = 0$  partial wave, we have  $\delta_0 = -ka$  [see eq. (4.181)], which can be made arbitrarily small by diminishing the quantity  $a$ . However the Born approximation is clearly inapplicable in this case, since  $U(r)$  is infinite at  $r = a$ .

## 8.6. Examples

### 8.6.1. The Yukawa potential

Let us first consider the Yukawa potential

$$U(r) = -U_0 e^{-ar}/r = -U_0 e^{-r/a}/r \quad (8.81)$$

where  $a = \alpha^{-1}$  is the "range" of the interaction.



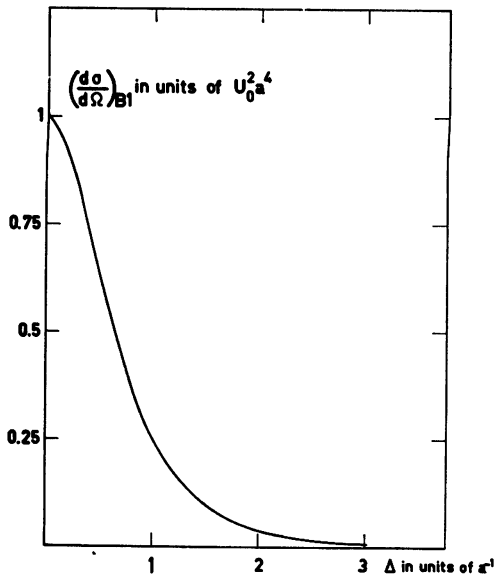


Fig. 8.2. The first Born differential cross section  $(d\sigma/d\Omega)_{B1}$ , measured in units of  $U_0^2 a^4$ , as a function of the wave vector transfer  $\Delta$  (measured in units of  $a^{-1}$ ) for a Yukawa potential (8.81).

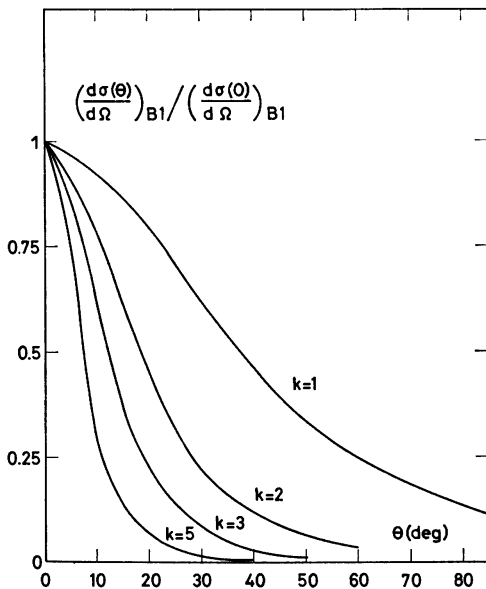


Fig. 8.3. The first Born angular distribution for scattering by a Yukawa potential (8.81) and for various values of the wave number  $k$  (measured in units of  $a^{-1}$ ).

The *first Born* scattering amplitude  $f_{B1}$  is given by eq. (8.9), namely

$$f_{B1} = -2\pi^2 \langle \Phi_{k_f} | U | \Phi_{k_i} \rangle = -2\pi^2 \langle k_f | U | k_i \rangle$$

or explicitly

$$f_{B1} = \frac{U_0}{\Delta} \int_0^\infty \sin(\Delta r) e^{-\alpha r} dr, \quad \Delta = 2k \sin \frac{1}{2}\theta \quad (8.82)$$

so that

$$f_{B1} = U_0/(\alpha^2 + \Delta^2). \quad (8.83)$$

The first Born differential scattering cross section is then

$$(d\sigma/d\Omega)_{B1} = U_0^2/(\alpha^2 + \Delta^2)^2. \quad (8.84)$$

We see that it is identical for an attractive ( $U_0 > 0$ ) or a repulsive ( $U_0 < 0$ ) potential having the same values of  $|U_0|$  and  $\alpha$ . The total first Born cross section is given by

$$\sigma_{tot}^{B1} = \frac{2\pi}{k^2} U_0^2 \int_0^{2k} \frac{\Delta}{(\alpha^2 + \Delta^2)^2} d\Delta \quad (8.85)$$

or

$$\sigma_{tot}^{B1} = \frac{4\pi U_0^2}{\alpha^2(\alpha^2 + 4k^2)}. \quad (8.86)$$

We verify that

$$\sigma_{tot}^{B1} \underset{k \rightarrow \infty}{\sim} A/E \quad (8.87)$$

where  $A = \pi \hbar^2 U_0^2 / 2m \alpha^2$  and  $E = \hbar^2 k^2 / 2m$  is the incident energy. The first Born differential cross section (8.84), measured in units of  $U_0^2 a^4$ , is shown in Fig. 8.2 as a function of the magnitude  $\Delta$  of the wave vector transfer (measured in units of  $a^{-1}$ ). We remark that it is a “universal” curve, valid for all Yukawa potentials. We also show in Fig. 8.3 the first Born angular distribution corresponding to the Yukawa potential (8.81) and for various choices of incident wave numbers  $k$  (measured in units  $a^{-1}$ ). We note that, at high energies, the scattering predicted by the Born approximation is essentially concentrated within a forward cone of angular range  $(ka)^{-1}$ . This behaviour follows directly from eq. (8.30) and the fact that the Fourier transform of a function  $U(r)$  which is negligible beyond  $r \simeq a$  is appreciable only for values of  $\Delta$  such that

$$\Delta \lesssim a^{-1} \quad (8.88)$$

i.e. [see eq. (8.29)] for scattering angles  $\theta$  given by

$$\theta \lesssim 1/ka. \quad (8.89)$$

For the Yukawa potential (8.66) describing approximately high energy elastic electron-atom scattering, we find that

$$f_{B1}(\Delta) = \frac{2Z}{a_0(a^{-2} + \Delta^2)}, \quad a_0 = \hbar^2/me^2 \quad (8.90)$$

so that the corresponding first Born differential cross section is given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{B1} = \frac{4Z^2}{a_0^2(a^{-2} + 4k^2 \sin^2 \frac{1}{2}\theta)^2}. \quad (8.91)$$

We note that when  $a \rightarrow \infty$  (no screening), we recover the Rutherford result (6.40), so that the *first Born approximation gives the correct differential cross section for the Coulomb potential*. When the quantity  $a$  is finite we see also that eq. (8.91), unlike the Rutherford formula, yields a finite result in the forward direction. The total cross section is then finite and given from eq. (8.86) by

$$\sigma_{\text{tot}}^{B1} = 16\pi Z^2 a^4 / \{a^2(4k^2 a^2 + 1)\}. \quad (8.92)$$

Using the Thomas-Fermi value (8.67) for  $a$ , we may obtain the asymptotic value of the first Born total cross section, namely

$$\sigma_{\text{tot}}^{B1} \underset{k \rightarrow \infty}{\sim} 4\pi Z^4 / k^2. \quad (8.93)$$

Let us now study the *second Born approximation* for the Yukawa potential. We have to evaluate the quantity  $\tilde{f}_{B2}$  which we write in momentum space as

$$\tilde{f}_{B2} = 2\pi^2 \int d\mathbf{k} \langle \mathbf{k}_f | U | \mathbf{k} \rangle \frac{1}{\kappa^2 - k^2 - i\varepsilon} \langle \mathbf{k} | U | \mathbf{k}_i \rangle \quad (8.94)$$

or, explicitly

$$\tilde{f}_{B2} = (2\pi^2)^{-1} U_0^2 \int d\mathbf{k} \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\alpha^2 + |\mathbf{k} - \mathbf{k}_i|^2)(\alpha^2 + |\mathbf{k} - \mathbf{k}_f|^2)} \quad (8.95)$$

where we have used the fact that

$$\langle \mathbf{q} | U | \mathbf{q}' \rangle = -U_0 / \{\alpha^2 + |\mathbf{q}' - \mathbf{q}|^2\} \quad (8.96)$$

for the Yukawa potential (8.81). The evaluation of the integral appearing on the right-hand side of eq. (8.95), together with that of more general *Dalitz integrals* [16, 17] of the form

$$I_{m,n}(\alpha, \beta; \mathbf{k}_i, \mathbf{k}_f; k) = \int d\mathbf{k} \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\alpha^2 + |\mathbf{k} - \mathbf{k}_i|^2)^m (\beta^2 + |\mathbf{k} - \mathbf{k}_f|^2)^n} \quad (m, n = 1, 2, \dots) \quad (8.97)$$

are discussed in Appendix D. One finds in this case

$$\begin{aligned} \tilde{f}_{B2}(k, \theta) &= \frac{U_0^2}{2k \sin \frac{1}{2}\theta [\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2}} \\ &\times \left\{ \tan^{-1} \frac{\alpha k \sin \frac{1}{2}\theta}{[\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2}} \right. \\ &\left. + \frac{1}{2}i \log \left[ \frac{[\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2} + 2k^2 \sin \frac{1}{2}\theta}{[\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2} - 2k^2 \sin \frac{1}{2}\theta} \right] \right\}. \quad (8.98) \end{aligned}$$

It is a simple matter to verify that  $\text{Im } \tilde{f}_{B2}(\theta = 0) = k\sigma_{\text{tot}}^{B1}/4\pi$ , in accordance with eq. (8.46). For further reference we also write  $\tilde{f}_{B2}$  as a function of  $k$  and  $\Delta$  as

$$\tilde{f}_{B2}(k, \Delta) = \frac{U_0^2}{\Delta[\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2]^{1/2}} \left\{ \tan^{-1} \frac{\alpha\Delta}{2[\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2]^{1/2}} + \frac{1}{2}i \log \left[ \frac{(\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2)^{1/2} + k\Delta}{(\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2)^{1/2} - k\Delta} \right] \right\}. \quad (8.99)$$

We also note from eq. (8.99) that if we let  $k$  become large we find that

$$\text{Re } \tilde{f}_{B2}(k, \Delta) = A(\Delta)/k^2 + \dots \quad (8.100)$$

while

$$\text{Im } \tilde{f}_{B2}(k, \Delta) = B(\Delta)/k + \dots \quad (8.101)$$

where the functions  $A(\Delta)$  and  $B(\Delta)$  only depend on  $\Delta$  and we have neglected terms of higher order in  $k^{-1}$ . We recall that  $f_{B1}$  is also a function of  $\Delta$  alone.

The second Born differential cross section is given by

$$(d\sigma/d\Omega)_{B2} = |f_{B2}|^2 = |f_{B1} + \tilde{f}_{B2}|^2 \quad (8.102)$$

TABLE 8.1

Differential scattering cross section for the Yukawa potential  $U(r) = -U_0 e^{-r}/r$  of the text with  $U_0 = 1$ . The notation  $6.22(-1)$  means  $6.22 \times 10^{-1}$

$k$ ( $a^{-1}$ )	$\theta$ (degrees)	First Born approximation	Second Born approximation	Exact
1	0	1.00	1.25	1.14
	30	6.22 (-1)	8.17 (-1)	7.31 (-1)
	60	2.50 (-1)	3.70 (-1)	3.21 (-1)
	90	1.11 (-1)	1.88 (-1)	1.59 (-1)
	120	6.25 (-2)	1.18 (-1)	9.84 (-2)
	150	4.47 (-2)	8.99 (-2)	7.49 (-2)
	180	4.00 (-2)	8.23 (-2)	6.86 (-2)
3	0	1.00	1.03	1.01
	30	8.59 (-2)	9.45 (-2)	8.91 (-2)
	60	1.00 (-2)	1.22 (-2)	1.07 (-2)
	90	2.77 (-3)	3.65 (-3)	3.02 (-3)
	120	1.28 (-3)	1.77 (-3)	1.40 (-3)
	150	8.36 (-4)	1.20 (-3)	9.24 (-4)
	180	7.30 (-4)	1.06 (-3)	8.09 (-4)
5	0	1.00	1.01	1.00
	30	1.69 (-2)	1.80 (-2)	1.72 (-2)
	60	1.48 (-3)	1.68 (-3)	1.53 (-3)
	90	3.84 (-4)	4.57 (-4)	3.99 (-4)
	120	1.73 (-4)	2.12 (-4)	1.80 (-4)
	150	1.12 (-4)	1.40 (-4)	1.17 (-4)
	180	9.80 (-5)	1.22 (-4)	1.02 (-4)

and we see that for large  $k$  it takes the form

$$\left(\frac{d\sigma}{d\Omega}\right)_{B2} = \left(f_{B1}(\Delta) + \frac{A(\Delta)}{k^2}\right)^2 + \frac{B^2(\Delta)}{k^2} \quad (8.103)$$

or, to order  $k^{-2}$ ,

$$\left(\frac{d\sigma}{d\Omega}\right)_{B2} = \left(\frac{d\sigma}{d\Omega}\right)_{B1} + \frac{1}{k^2}[2f_{B1}(\Delta)A(\Delta) + B^2(\Delta)]. \quad (8.104)$$

TABLE 8.2

Differential scattering cross section for the Yukawa potential  $U(r) = -U_0 e^{-r}/r$  of the text with  $U_0 = 5$

$k$ ( $a^{-1}$ )	$\theta$ (degrees)	First Born approximation	Second Born approximation	Exact
1	0	2.50 (+1)	8.13 (+1)	1.14 (+1)
	30	1.56 (+1)	6.31 (+1)	5.49
	60	6.25	4.03 (+1)	1.02
	90	2.78	2.75 (+1)	6.87 (−1)
	120	1.56	2.09 (+1)	1.71
	150	1.12	1.77 (+1)	2.77
	180	1.00	1.67 (+1)	3.20
3	0	2.50 (+1)	3.26 (+1)	2.05
	30	2.15	5.01	1.64
	60	2.50 (−1)	1.19	2.39 (−1)
	90	6.93 (−2)	4.90 (−1)	8.45 (−2)
	120	3.19 (−2)	2.80 (−1)	4.59 (−2)
	150	2.09 (−2)	2.05 (−1)	3.31 (−2)
	180	1.83 (−2)	1.85 (−1)	2.98 (−2)
5	0	2.50 (+1)	2.78 (+1)	2.31 (+1)
	30	4.22 (−1)	8.83 (−1)	3.98 (−1)
	60	3.70 (−2)	1.37 (−1)	3.98 (−2)
	90	9.61 (−3)	4.74 (−2)	1.10 (−2)
	120	4.33 (−3)	2.50 (−2)	5.14 (−3)
	150	2.81 (−3)	1.76 (−2)	3.39 (−3)
	180	2.45 (−3)	1.57 (−2)	2.97 (−3)

In order to check how accurate the *first* and *second* Born approximations are in the case of a Yukawa potential, we compare in Table 8.1 the differential cross sections  $(d\sigma/d\Omega)_{B1}$  and  $(d\sigma/d\Omega)_{B2}$  (obtained respectively from eqs. (8.84) and (8.102)) with the *exact* results (calculated by using the partial wave method and computing the phase shifts by numerical integration of the radial Schrödinger equations). This comparison is made for an attractive Yukawa potential of unit “range”  $a = \alpha^{-1}$  [18] and having a “strength”  $U_0 = 1$ . The results are given for three values of the wave number ( $k = 1, 3, 5$ , in units  $a^{-1}$ ) and various scattering angles.

A look at Table 8.1 shows that except at the lowest value of  $k$  the second Born approximation offers no improvement over the first Born values. The results at  $k = 5$  are particularly discouraging since we would expect the Born series to converge quickly in this case for which  $|U_0|a/2k = 1/10$ .

The reason for this failure of the second Born approximation may be found by returning to eq. (8.104) and noting that this formula does not provide *all* the corrections of order  $k^{-2}$  to the first Born *cross section*. In fact, one may show [19] that the *real* part of the *third* order term  $f_{B3}$  of the Born series also

TABLE 8.3

Differential scattering cross section for the Yukawa potential  $U(r) = -U_0 e^{-r}/r$  of the text with  $U_0 = 0.2$

$k$ ( $a^{-1}$ )	$\theta$ (degrees)	First Born approximation	Second Born approximation	Exact
1	0	4.00 (−2)	4.17 (−2)	4.16 (−2)
	30	2.49 (−2)	2.61 (−2)	2.61 (−2)
	60	1.00 (−2)	1.07 (−2)	1.07 (−2)
	90	4.44 (−3)	4.87 (−3)	4.83 (−3)
	120	2.50 (−3)	2.78 (−3)	2.75 (−3)
	150	1.79 (−3)	2.01 (−3)	1.99 (−3)
	180	1.60 (−3)	1.80 (−3)	1.78 (−3)
3	0	4.00 (−2)	4.02 (−2)	4.02 (−2)
	30	3.44 (−3)	3.48 (−3)	3.47 (−3)
	60	4.00 (−4)	4.09 (−4)	4.07 (−4)
	90	1.11 (−4)	1.14 (−4)	1.13 (−4)
	120	5.10 (−5)	5.26 (−5)	5.20 (−5)
	150	3.34 (−5)	3.46 (−5)	3.41 (−5)
	180	2.92 (−5)	3.02 (−5)	2.98 (−5)
5	0	4.00 (−2)	4.01 (−2)	4.01 (−2)
	30	6.75 (−4)	6.80 (−4)	6.79 (−4)
	60	5.92 (−5)	5.98 (−5)	5.96 (−5)
	90	1.54 (−5)	1.56 (−5)	1.55 (−5)
	120	6.93 (−6)	7.03 (−6)	6.98 (−6)
	150	4.50 (−6)	4.57 (−6)	4.53 (−6)
	180	3.92 (−6)	3.98 (−6)	3.95 (−6)

gives a contribution of order  $k^{-2}$  (for large  $k$ ) to the scattering amplitude and therefore also to the differential cross section. The second Born cross section (8.104) lacks this term [20] which is of third order in the potential (i.e. proportional to  $U_0^3$ ). We note that the importance of this missing term with respect to the contribution coming from  $\text{Re } f_{B2}$  should increase with the “strength”  $|U_0|$  of the potential. This is illustrated by Tables 8.2 and 8.3 which correspond respectively to the choices  $U_0 = 5$  and  $U_0 = 0.2$  of the potential strength. The second Born results are seen to be disastrous in Table 8.2; they are much better in Table 8.3.

It is important to remark that the above comments do not contradict the convergence criteria for the Born series discussed in Section 8.4, since these criteria apply to the *wave function* or the *scattering amplitude*, not the *cross sections*. If we denote by  $f$  the exact scattering amplitude, the convergence criteria only tell us that the quantities  $|f - f_{B1}|$ ,  $|f - f_{B2}|$ , etc. . . . are getting progressively smaller in the convergence domain.

We have pointed out in Section 8.5 that the Born series may also be used for the computation of the phase shifts. As an example, we compare in Table 8.4 the first Born results for  $\tan \delta_l$  with the exact ones [obtained by integrating numerically the radial equation (4.17) and using eq. (4.113)] for two attractive Yukawa potentials (8.81) having a unit "range"  $a = 1$  and strength parameters  $U_0 = 1$  and  $U_0 = 20$ , respectively. This comparison is made for various values of  $l$  and for a wave number  $k = 5$ . We note that for the case  $U_0 = 1$  (such that  $|U_0|a/2k = 1/10$ ), the first Born values are very

TABLE 8.4

Comparison of the quantity  $\tan \delta_l$ , as obtained from the first Born approximation [see eq. (8.74)] and from the "exact" formula (4.113), for attractive Yukawa potentials of the form  $U(r) = -U_0 e^{-r}/r$  and for various values of  $l$ . The wave number is  $k = 5$ . The numbers in parentheses indicate powers of 10.

$l$	$U_0 = 1$		$U_0 = 20$	
	Born	Exact	Born	Exact
0	2.31 (-1)	2.38 (-1)	4.62	2.21
1	1.35 (-1)	1.38 (-1)	2.71	-9.23 (-2)
2	9.17 (-2)	9.28 (-2)	1.83	-1.55
3	6.57 (-2)	6.63 (-2)	1.31	1.97 (+1)
4	4.85 (-2)	4.88 (-2)	9.70 (-1)	1.95
5	3.65 (-2)	3.66 (-2)	7.29 (-1)	1.05
10	1.01 (-2)	1.01 (-2)	2.02 (-1)	2.12 (-1)
15	3.10 (-3)	3.10 (-3)	6.20 (-2)	6.29 (-2)
20	1.00 (-3)	1.00 (-3)	2.00 (-2)	2.01 (-2)

accurate, even for the lowest partial waves. Indeed, the largest discrepancy (which occurs in the s-wave) is only about 3%. For the stronger coupling case  $U_0 = 20$  such that  $|U_0|a/2k = 2$ , the first Born and exact results disagree for the lowest  $l$ -values, but come progressively close together as  $l$  increases and the centrifugal barrier  $l(l+1)/r^2$  keeps the particle away from the interaction region. In fact, for  $l = 10$  we see that the first Born and exact results already agree very well (within 5%). This is in accordance with the discussion of Section 4.3.4.

Finally, we display in Table 8.5 the total first Born cross sections which we compare with the exact results for the choice  $U_0 = 2$  and several values of  $k$ . It is interesting to note that the first Born values are more accurate than expected at the lowest values of  $k$ . This is also true for the first Born differential cross sections given in Tables 8.1–8.3.

TABLE 8.5

Total cross section for the Yukawa potential  $U(r) = -U_0 e^{-r}/r$ , with  $U_0 = 2$ . The unit of length is the "range" of the potential

$k$	First Born approximation	Exact
1	10.0	12.4
2	2.96	3.12
3	1.36	1.39
4	7.73 (-1)	7.85 (-1)
5	4.98 (-1)	5.02 (-1)
6	3.47 (-1)	3.49 (-1)
7	2.55 (-1)	2.56 (-1)
8	1.96 (-1)	1.96 (-1)
9	1.55 (-1)	1.55 (-1)
10	1.25 (-1)	1.25 (-1)

### 8.6.2. Superposition of Yukawa potentials

The calculations made above for a simple Yukawa potential are easily generalized to include superposition of Yukawa potentials of the form

$$U(r) = -U_0 \int_{v_0 > 0}^{\infty} \rho(v) \frac{e^{-vr}}{r} dv \quad (8.105)$$

where the weight function  $\rho(v)$  is bounded everywhere except perhaps for delta-function singularities. The "range" of the potential (8.105) is simply  $v_0^{-1}$ . Interactions of the form (8.105) are of interest in strong interaction physics.

The first Born scattering amplitude is readily obtained from eq. (8.9); it is given by

$$f_{B1} = U_0 \int_{v_0}^{\infty} \frac{\rho(v)}{v^2 + \Delta^2} dv \quad (8.106)$$

and obviously reduces to eq. (8.83) when  $\rho(v) = \delta(v - \alpha)$ .

The second Born approximation to the scattering amplitude is  $f_{B2} = f_{B1} + \bar{f}_{B2}$ , with

$$\begin{aligned} \bar{f}_{B2} = & (2\pi^2)^{-1} U_0^2 \int_{v_0}^{\infty} d\mu \rho(\mu) \int_{v_0}^{\infty} dv \rho(v) \\ & \times \int d\mathbf{k} \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\mu^2 + |\mathbf{k} - \mathbf{k}_i|^2)(v^2 + |\mathbf{k} - \mathbf{k}_f|^2)} \end{aligned} \quad (8.107)$$

an expression which generalizes eq. (8.95). Following the method of Appendix D, we find that

$$\bar{f}_{B2} = -\frac{U_0^2}{2} \int_{v_0}^{\infty} d\mu \rho(\mu) \int_{v_0}^{\infty} dv \rho(v) \int_0^1 \frac{dt}{\Gamma[2ik\Gamma - \mu^2 t - v^2(1-t)]} \quad (8.108)$$



with

$$\Gamma^2 = \mu^2 t + v^2(1 - t) + t(1 - t)\Delta^2. \quad (8.109)$$

Instead of analyzing in detail the expression (8.108), we shall simply obtain for further reference the leading term of  $\tilde{f}_{B2}$  for large  $k$ . Thus we write in this case

$$\tilde{f}_{B2} = \frac{iU_0^2}{4k} \int_{v_0}^{\infty} d\mu \rho(\mu) \int_{v_0}^{\infty} dv \rho(v) \int_0^1 \frac{dt}{\mu^2 t + v^2(1 - t) + t(1 - t)\Delta^2} + \dots \quad (8.110)$$

where higher order terms in  $k^{-1}$  have been neglected. The  $t$ -integral may be done in closed form [21] and yields

$$\int_0^1 \frac{dt}{v^2 + (\mu^2 - v^2 + \Delta^2)t - \Delta^2 t^2} = \frac{1}{\mu v \sqrt{u^2 - 1}} \log[u + \sqrt{u^2 - 1}] \quad (8.111)$$

where

$$u = \frac{\mu^2 + v^2 + \Delta^2}{2\mu v} \quad (8.112)$$

so that

$$\tilde{f}_{B2} = i \frac{U_0^2}{4k} \int_{v_0}^{\infty} d\mu \rho(\mu) \int_{v_0}^{\infty} dv \rho(v) \frac{1}{\mu v \sqrt{u^2 - 1}} \log[u + \sqrt{u^2 - 1}] + \dots \quad (8.113)$$

We note that the leading term of  $\tilde{f}_{B2}$  for large  $k$  is imaginary and of order  $k^{-1}$ , as for the simple Yukawa potential [(see eq. (8.101)]. The real part of  $\tilde{f}_{B2}$  may also be shown to be of order  $k^{-2}$  and to have the form given by eq. (8.100). The comments made in Section 8.6.1 about the second Born approximation also apply in this case.

In order to illustrate our discussion, we consider a particular superposition of two Yukawa potentials of different ranges, namely [22]

$$U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r. \quad (8.114)$$

Potentials of this kind, which may simulate a short-range repulsive and long-range attractive behaviour (or vice-versa) can be used to reproduce some of the features of strong interaction forces [e.g. 23]. We note that the first Born approximation amplitude

$$f_{B1}(\Delta) = U_0 \left[ \frac{1}{1 + \Delta^2} - 1.125 \frac{1}{4 + \Delta^2} \right] \quad (8.115)$$

may already exhibit a non-trivial structure since it vanishes for  $\Delta \simeq 4.8$ . Because the maximum value of  $\Delta$  (reached for  $\theta = \pi$ ) is  $\Delta_{\max} = 2k$ , we see that  $f_{B1}(\Delta)$ , as given by eq. (8.115), will change sign in the "physical region"  $0 \leq \Delta \leq 2k$  as soon as  $k \geq 2.4$ .

TABLE 8.6

Differential scattering cross section for the "double Yukawa" potential

$$U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r \text{ of the text with } U_0 = 1.$$

The wave number is  $k = 5$ 

$\theta$ (degrees)	First Born approximation	Second Born approximation	Exact
0	5.17 (-1)	5.18 (-1)	5.17 (-1)
30	6.12 (-4)	6.08 (-4)	6.03 (-4)
60	1.10 (-7)	1.60 (-7)	1.63 (-7)
90	1.50 (-6)	1.54 (-6)	1.52 (-6)
120	1.17 (-6)	1.17 (-6)	1.16 (-6)
150	9.17 (-7)	9.12 (-7)	9.03 (-7)
180	8.40 (-7)	8.33 (-7)	8.24 (-7)

TABLE 8.7

Differential scattering cross section for the "double Yukawa" potential

$$U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r \text{ of the text with } U_0 = 5.$$

The wave number is  $k = 5$ 

$\theta$ (degrees)	First Born approximation	Second Born approximation	Exact
0	1.29 (+1)	1.32 (+1)	1.29 (+1)
30	1.53 (-2)	1.76 (-2)	1.47 (-2)
60	2.75 (-6)	1.22 (-5)	1.35 (-5)
90	3.75 (-5)	4.88 (-5)	4.00 (-5)
120	2.93 (-5)	3.56 (-5)	2.80 (-5)
150	2.29 (-5)	2.71 (-5)	2.11 (-5)
180	2.10 (-5)	2.45 (-5)	1.91 (-5)

TABLE 8.8

Differential scattering cross section for the "double Yukawa" potential

$$U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r \text{ of the text with } U_0 = 0.2.$$

The wave number is  $k = 5$ 

$\theta$ (degrees)	First Born approximation	Second Born approximation	Exact
0	2.07 (-2)	2.07 (-2)	2.07 (-2)
30	2.45 (-5)	2.44 (-5)	2.44 (-5)
60	4.40 (-9)	4.76 (-9)	4.78 (-9)
90	6.01 (-8)	6.03 (-8)	6.03 (-8)
120	4.69 (-8)	4.68 (-8)	4.68 (-8)
150	3.67 (-8)	3.66 (-8)	3.66 (-8)
180	3.36 (-8)	3.35 (-8)	3.34 (-8)

We give in Tables 8.6, 8.7 and 8.8 a detailed comparison of the first and second Born differential cross sections with the corresponding exact results, for a wave number  $k = 5$  and the three values  $U_0 = 1, 5$  and  $0.2$  of the "strength" parameter  $U_0$ . The comments made about Tables 8.1–8.3 apply equally here, but the second Born approximation is nevertheless seen to be more accurate in the present case. This is undoubtedly due to the fact that the potential (8.114) is less "strong" than a corresponding simple Yukawa potential with the same value of  $U_0$  [24].

### 8.6.3. The separable non local potential [25]

The Born series which we have discussed so far in the case of local interactions is readily generalized to include non-local potentials  $\langle \mathbf{r}|U|\mathbf{r}' \rangle$ . The basic equations (8.12) and (8.14) are still valid, and we have now explicitly [compare with eq. (8.39)]

$$\begin{aligned} \tilde{f}_{Bj} = & -\frac{1}{4\pi} \int d\mathbf{r}_1 d\mathbf{r}'_1 \dots d\mathbf{r}_j d\mathbf{r}'_j \exp(-i\mathbf{k}_f \cdot \mathbf{r}_1) \langle \mathbf{r}_1|U|\mathbf{r}'_1 \rangle G_0^{(+)}(\mathbf{r}'_1, \mathbf{r}_2) \\ & \times \langle \mathbf{r}_2|U|\mathbf{r}'_2 \rangle \dots G_0^{(+)}(\mathbf{r}'_{j-1}, \mathbf{r}_j) \langle \mathbf{r}_j|U|\mathbf{r}'_j \rangle \exp(i\mathbf{k}_i \cdot \mathbf{r}'_j). \end{aligned} \quad (8.116)$$

In momentum space we may use directly eqs. (8.41) and (8.42) if we replace eq. (8.40) by the more general definition

$$\langle \mathbf{q}|U|\mathbf{q}' \rangle = (2\pi)^{-3} \int d\mathbf{r} d\mathbf{r}' \exp(-i\mathbf{q} \cdot \mathbf{r}) \langle \mathbf{r}|U|\mathbf{r}' \rangle \exp(i\mathbf{q}' \cdot \mathbf{r}'). \quad (8.117)$$

We note that eqs. (8.116) and (8.117) reduce to eqs. (8.39) and (8.40), respectively, when  $\langle \mathbf{r}|U|\mathbf{r}' \rangle = U(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')$ .

As an example of non-local interaction, let us consider the separable non-local potential (5.149), namely

$$\langle \mathbf{r}|U|\mathbf{r}' \rangle = \lambda u(\mathbf{r})u(\mathbf{r}') \quad (8.118)$$

for which the exact amplitude is given by eq. (5.154).

The first Born approximation, given by eq. (8.41), is simply

$$f_{B1} = -\frac{\lambda}{4\pi} \int d\mathbf{r} \exp(-i\mathbf{k}_f \cdot \mathbf{r}) u(\mathbf{r}) \int d\mathbf{r}' u(\mathbf{r}') \exp(i\mathbf{k}_i \cdot \mathbf{r}') \quad (8.119)$$

where we have used eqs. (8.117) and (8.118). Introducing the Fourier transform of the function  $u(\mathbf{r})$ , namely

$$\tilde{u}(\mathbf{q}) = (2\pi)^{-3/2} \int \exp(i\mathbf{q} \cdot \mathbf{r}) u(\mathbf{r}) d\mathbf{r} \quad (8.120)$$

we simply have

$$f_{B1} = -2\pi^2 \lambda \tilde{u}(-\mathbf{k}_f) \tilde{u}(\mathbf{k}_i). \quad (8.121)$$

Let us choose the function  $u(\mathbf{r}) \equiv u(r) = (\pi/2)^{1/2} \exp(-\beta r)/r$  so that its Fourier transform  $\tilde{u}(\mathbf{q})$  assumes the simple form

$$\tilde{u}(\mathbf{q}) = (q^2 + \beta^2)^{-1}. \quad (8.122)$$

We shall call the corresponding separable potential the *Yamaguchi potential* [26]. Then we find that

$$f_{B1} = -2\pi^2\lambda(k^2 + \beta^2)^{-2}. \quad (8.123)$$

In contrast with the Yukawa potential studied previously, we note that  $f_{B1}$  is of order  $k^{-4}$  for large  $k$ .

The second Born approximation  $f_{B2}$  for the scattering amplitude is given by  $f_{B2} = f_{B1} + \tilde{f}_{B2}$ , where according to eq. (8.42),

$$\tilde{f}_{B2} = 2\pi^2 \int d\mathbf{k} \frac{1}{\kappa^2 - k^2 - i\varepsilon} \langle \mathbf{k}_f | U | \mathbf{k} \rangle \langle \mathbf{k} | U | \mathbf{k}_i \rangle. \quad (8.124)$$

Hence, for the Yamaguchi potential corresponding to the choice (8.122), we have

$$\tilde{f}_{B2} = 2\pi^2\lambda^2(k^2 + \beta^2)^{-2} \int d\mathbf{k} \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\kappa^2 + \beta^2)^2}. \quad (8.125)$$

The integral on the right-hand side of eq. (8.125) is just a particular case of the quantity  $L_2(k, \Gamma, A)$  calculated in Appendix D. With  $\Gamma = \beta$  and  $A = 0$ , we find that

$$\tilde{f}_{B2} = 2\pi^2\lambda^2(k^2 + \beta^2)^{-2} \left[ -\frac{\pi^2}{\beta(k^2 - \beta^2 + 2ik\beta)} \right] \quad (8.126)$$

and therefore

$$f_{B2} = f_{B1} \left[ 1 + \frac{\lambda\pi^2}{\beta(k^2 - \beta^2 + 2ik\beta)} \right]. \quad (8.127)$$

We note that for large  $k$  the quantity  $\text{Re } \tilde{f}_{B2}$  is of order  $k^{-6}$ , while  $\text{Im } \tilde{f}_{B2}$  is of order  $k^{-7}$ . These results are again in marked contrast with those found for the Yukawa potential.

Consider now the *exact* scattering amplitude given by eq. (5.40). We see from eq. (5.154) that for a separable potential this expression may be written as

$$f = f_{B1}[1 - \tilde{f}_{B2}/f_{B1}]^{-1}. \quad (8.128)$$

The Born series for the scattering amplitude is simply obtained by expanding the quantity  $[1 - \tilde{f}_{B2}/f_{B1}]^{-1}$  in eq. (8.128) as  $[1 - x]^{-1} = 1 + x + x^2 + \dots$ . Returning to the case of the Yamaguchi potential, we find from eq. (8.128) that

$$f = f_{B1} \left[ 1 - \frac{\lambda\pi^2}{\beta(k^2 - \beta^2 + 2ik\beta)} \right]^{-1} \quad (8.129)$$

an expression which is independent of the scattering angle  $\theta$  as the Yamaguchi interaction only acts in the s-state. We verify that the first Born approximation yields the correct result in the limit  $k \rightarrow \infty$ , but is only satisfactory at low energies ( $k \rightarrow 0$ ) if

$$|\lambda| \ll \pi^{-2}\beta^3 \quad (8.130)$$

i.e. for a very "weak" potential. More generally, the convergence of the Born series will be ensured if

$$\frac{|\lambda|\pi^2}{\beta} \left| \frac{1}{k^2 - \beta^2 + 2ik\beta} \right| < 1 \quad (8.131)$$

or

$$k^2 > \beta^{-1}(|\lambda|\pi^2 - \beta^3). \quad (8.132)$$

Two cases must be considered:

1) If the quantity  $|\lambda|$  is such that

$$|\lambda| < \pi^{-2}\beta^3 \quad (8.133)$$

the condition (8.131) is fulfilled for any physical value of  $k$ . The convergence relation (8.133) is naturally less restrictive than the validity condition (8.130) of the first Born approximation at low energies. One can easily show also that the convergence condition (8.133) implies that the separable potential

$$\langle \mathbf{r}|U|\mathbf{r}' \rangle = -\lambda_0 u(\mathbf{r})u(\mathbf{r}'), \quad \lambda_0 > 0 \quad (8.134)$$

cannot support a bound state. For example, if the Yamaguchi potential [such that  $u(\mathbf{r}) = (\pi/2)^{1/2} \exp(-\beta r)/r$ ] has a bound state of energy  $\varepsilon = -\hbar^2\alpha^2/2m$  one finds [26] that the corresponding parameter  $\lambda_0$  is given by

$$\lambda_0 = \pi^{-2}\beta(\alpha + \beta)^2, \quad \alpha, \beta > 0. \quad (8.135)$$

Hence the condition (8.133) [which now reads  $\lambda_0 < \pi^{-2}\beta^3$ ] is never satisfied.

2) On the contrary, if

$$|\lambda| > \pi^{-2}\beta^3 \quad (8.136)$$

the condition (8.132) becomes

$$k > k_0 = (|\lambda|\pi^2/\beta - \beta^2)^{1/2} \quad (8.137)$$

so that the Born series will only converge for  $k > k_0$ .

We have thus far examined the first Born amplitude (8.123), the second Born expression (8.127) and the exact expression (8.129). We may of course readily obtain the higher Born terms by expanding the exact amplitude in powers of  $\lambda$ . For example, the third Born approximation  $f_{B3}$  is given by  $f_{B3} = f_{B1} + \bar{f}_{B2} + \bar{f}_{B3}$ , where

$$\bar{f}_{B3} = f_{B1} \frac{\lambda^2 \pi^4}{\beta^2(k^2 - \beta^2 + 2ik\beta)^2} \quad (8.138)$$

so that

$$f_{B3} = f_{B1} \left[ 1 + \frac{\lambda \pi^2}{\beta(k^2 - \beta^2 + 2ik\beta)} + \frac{\lambda^2 \pi^4}{\beta^2(k^2 - \beta^2 + 2ik\beta)^2} \right]. \quad (8.139)$$

We see that for large  $k$  the quantity  $\text{Re } \bar{f}_{B3}$  behaves like  $k^{-8}$  while  $\text{Im } \bar{f}_{B3}$  is

proportional to  $k^{-9}$ . Thus for large  $k$  the scattering amplitude takes the form

$$f = \underbrace{\lambda \frac{A}{k^4}}_{\mathcal{F}_{B1}} + \underbrace{\lambda^2 \left( \frac{B}{k^6} + i \frac{C}{k^7} \right)}_{\mathcal{F}_{B2}} + \underbrace{\lambda^3 \left( \frac{D}{k^8} + i \frac{E}{k^9} \right)}_{\mathcal{F}_{B3}} + \cdots \quad (8.140)$$

where  $A, B, C, D$  and  $E$  are constants. In particular, we note that the second Born amplitude  $\mathcal{F}_{B2}$  gives correctly the leading contribution to the imaginary part of the scattering amplitude (as for the Yukawa potential) but also the *two* leading terms of the real part (in contrast with the Yukawa case [27]). It is worth recalling in connection with the above equations that the Yamaguchi potential is a very particular interaction which only acts in the s-wave.

## References and notes

- [1] Some approximation methods are inherently of a many-body nature and cannot be introduced within the framework of potential scattering. This is the case for example of the *impulse approximation* which will be discussed in Chapter 19.
- [2] The first Born approximation is often called simply the Born approximation. It is due to BORN, M. (1926), *Z. f. Physik* **38**, 803.
- [3] Instead of calling the quantity  $\Delta$  “the magnitude of the wave vector transfer”, we shall frequently refer to it simply as “the wave vector transfer” or even “the momentum transfer” (these being equal in units such that  $\hbar = 1$ ).
- [4] JOST, R. and A. PAIS (1951), *Phys. Rev.* **82**, 840.
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- [6] ZEMACH, C. and A. KLEIN (1958), *Nuovo Cimento* **10**, 1078.
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- [9] MANNING, I. (1965), *Phys. Rev.* **139**, B 495.
- [10] SMITHIES, F. (1958), *Integral Equations* (Cambridge Univ. Press, New York) Chapter 2.
- [11] We note that eq. (8.50) may also be written as  $\lambda \|K\| < 1$  where  $\|K\|$  is the norm of the kernel  $K(x, y)$ , as defined in eq. (5.106).
- [12] BARGMANN, V. (1952), *Proc. Nat. Acad. Sc. U.S.* **38**, 961.
- [13] Remember that we are considering here only *non-relativistic* scattering. This conclusion does not necessarily hold for relativistic scattering.
- [14] This description of elastic electron-atom scattering by means of a “static” potential clearly ignores many-body effects, in particular exchange effects between the incident and atomic electrons. A detailed analysis of electron-atom scattering will be given in Chapters 19, 20 and 21.
- [15] The atomic velocity of an electron in the “first Bohr orbit” of an hydrogen-like atom of atomic number  $Z$  is  $v_0 = Ze^2/\hbar = Z\alpha c$  where  $\alpha = e^2/\hbar c \simeq 1/137$  is the fine structure constant.
- [16] DALITZ, R. H. (1961), *Proc. Roy. Soc.* **A206**, 509.
- [17] MORSE, P. M. and H. FESHBACH (1953), *Methods of Theoretical Physics* (McGraw-Hill, New York) Chapter 9.
- [18] This involves no loss of generality, since the “range”  $a$  may always be “factored out” of the problem by an appropriate choice of units.
- [19] We shall return to this point in Chapter 9.

- [20] Incidentally, we note that since the missing term of order  $k^{-2}$  arises from the *real* part of  $\tilde{f}_{B3}$ , it is the quantity  $\text{Re } f_{B2}$  which is in error. A detailed examination of the scattering amplitude indeed shows that  $\text{Im } f_{B2}$  is a better approximation to the exact quantity  $\text{Im } f$  than  $\text{Re } f_{B2}$  is to the exact value  $\text{Re } f$  when  $k$  is large.
- [21] GRADSHTEYN, I. S. and I. W. RYZHIK (1965), *Table of Integrals, Series and Products* (Academic Press, New York) formula (2.172).
- [22] The "range" of the first Yukawa potential in eq. (8.114) is chosen as the unit of length.
- [23] BALI, N. F., SHU-YUAN CHU, R. W. HAYMAKER and CHUNG-I TAN (1967), *Phys. Rev.* **161**, 1450.
- [24] A simple way to see this is to note that for the Yukawa potential (8.81) we have  $\max|rU(r)| = U_0$ , while for the interaction (8.114) we find that  $\max|rU(r)| = 2U_0/9$ .
- [25] We follow here the discussion of JOACHAIN, C. J. (1965), *Nucl. Phys.* **64**, 529.
- [26] YAMAGUCHI, Y. (1954), *Phys. Rev.* **95**, 1628.
- [27] We recall here the discussion following eq. (8.104).

## Semi-Classical Approximations

Semi-classical methods are useful approximation techniques when the de Broglie wavelength  $\lambda = h/p$  of the incident particle is sufficiently short compared with the distance in which the potential varies appreciably. If the potential has a “range”  $a$ , this *short wavelength* condition is equivalent to the requirement that  $ka \gg 1$ . We shall first study in Section 9.1 the *eikonal approximation* which originated in optics [1]. The eikonal scattering wave function is derived from the Lippmann–Schwinger equation by a linearization of the Green’s function in momentum space. The eikonal scattering amplitude and cross sections are then obtained and their properties are discussed. In particular, it is shown that the eikonal approximation, within its range of validity, satisfies the *optical theorem*. We also make a detailed comparison between the eikonal approximation and the Born series. Section 9.2 is devoted to the study of the Wentzel–Kramers–Brillouin or *W.K.B. method* in the simple case of the scattering by a central potential. We first recall the classical limit of the Schrödinger equation. We then obtain the W.K.B. radial wave functions, the corresponding phase shifts and the scattering amplitude.

### 9.1. The eikonal approximation

Originally introduced in quantum scattering theory by Molière [2], the eikonal approximation has been considerably developed by Glauber [3] who proposed a very fruitful many-body generalization of the method. We shall study in this section the essential features of this approximation, as applied



to the simple problem of non-relativistic potential scattering. A few other papers dealing with various aspects of the eikonal approximation are listed in references [4–23]. The application of the eikonal method to many-body scattering problems will be considered in Chapters 19, 20 and 21.

### 9.1.1. The eikonal scattering wave function [24]

Let us consider high-energy, non-relativistic potential scattering. We assume that  $ka \gg 1$  (the short wavelength condition) and also that  $|V_0|/E \ll 1$ , where  $|V_0|$  is a typical “strength” of the potential. We denote by  $|U_0|$  the corresponding “strength” of the reduced potential  $U(\mathbf{r}) = 2mV(\mathbf{r})/\hbar^2$ . We start from the Lippmann–Schwinger equation (5.33), namely

$$\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}') d\mathbf{r}' \quad (9.1)$$

where the Green’s function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  is given by

$$\begin{aligned} G_0^{(+)}(\mathbf{r}, \mathbf{r}') &= -\frac{1}{4\pi} \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \\ &= -(2\pi)^{-3} \lim_{\varepsilon \rightarrow 0^+} \int d\mathbf{k} \frac{\exp\{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')\}}{\kappa^2 - k^2 - i\varepsilon}. \end{aligned} \quad (9.2)$$

Since the potential varies slowly over the scale of the incident wavelength it is natural to factor out the free incident plane wave from the wave function  $\psi_{\mathbf{k}_i}^{(+)}$  and to write

$$\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \phi(\mathbf{r}) \quad (9.3)$$

where  $\phi(\mathbf{r})$  is a slowly varying function when  $ka$  is large. Substituting the ansatz (9.3) in eq. (9.1) we find that the function  $\phi(\mathbf{r})$  satisfies the equation

$$\phi(\mathbf{r}) = 1 - (2\pi)^{-3} \int d\mathbf{R} \int d\mathbf{k} \frac{\exp\{i(\mathbf{k} - \mathbf{k}_i) \cdot \mathbf{R}\}}{\kappa^2 - k^2 - i\varepsilon} U(\mathbf{r} - \mathbf{R}) \phi(\mathbf{r} - \mathbf{R}) \quad (9.4)$$

where we have set  $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ . This equation is still exact since eq. (9.3) merely defines the new function  $\phi(\mathbf{r})$ . However, it is now an easy matter to obtain an approximate form of  $\phi(\mathbf{r})$  by using the fact that the product  $U\phi$  varies slowly on the scale of the incident wavelength. In order to derive this result, let us first analyze the free propagator  $G_0^{(+)}$ . Using its representation in wave vector space which we recalled in eq. (9.2), and introducing the new variable

$$\mathbf{p} = \mathbf{k} - \mathbf{k}_i \quad (9.5)$$

we find that

$$G_0^{(+)}(\mathbf{R}) = -(2\pi)^{-3} \exp(i\mathbf{k}_i \cdot \mathbf{R}) \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{2\mathbf{k}_i \cdot \mathbf{p} + p^2 - i\varepsilon} \quad (9.6)$$

where the limiting process  $\varepsilon \rightarrow 0^+$  is always implied. We may therefore write eq. (9.4) as

$$\phi(\mathbf{r}) = 1 - I(\mathbf{r}) \quad (9.7)$$

where

$$I(\mathbf{r}) = (2\pi)^{-3} \int d\mathbf{R} \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{2\mathbf{k}_i \cdot \mathbf{p} + p^2 - i\varepsilon} U(\mathbf{r} - \mathbf{R}) \phi(\mathbf{r} - \mathbf{R}). \quad (9.8)$$

Since the product  $U\phi$  is slowly varying, this integral is dominated by small values of  $p/k$ . We may therefore expand [8] the quantity  $(2\mathbf{k}_i \cdot \mathbf{p} + p^2 - i\varepsilon)^{-1}$  in powers of  $p/k$  as

$$\begin{aligned} \frac{1}{2\mathbf{k}_i \cdot \mathbf{p} + p^2 - i\varepsilon} &= \frac{1}{2kp_z + p^2 - i\varepsilon} \\ &= \frac{1}{2kp_z - i\varepsilon} \left( 1 - \frac{1}{2kp_z - i\varepsilon} p^2 + \cdots \right) \end{aligned} \quad (9.9)$$

where we have chosen the  $z$ -axis in the direction of the incident wave vector  $\mathbf{k}_i$ . Accordingly, we may also write

$$G_0^{(+)}(\mathbf{R}) = G_0^{(1)}(\mathbf{R}) + G_0^{(2)}(\mathbf{R}) + \cdots \quad (9.10)$$

and

$$I(\mathbf{r}) = I^{(1)}(\mathbf{r}) + I^{(2)}(\mathbf{r}) + \cdots \quad (9.11)$$

Here

$$G_0^{(1)}(\mathbf{R}) = - (2\pi)^{-3} \exp(i\mathbf{k}_i \cdot \mathbf{R}) \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{2kp_z - i\varepsilon} \quad (9.12)$$

is the Green's function which corresponds to a *linearized propagator*, obtained by neglecting the term  $p^2$  in the expression  $(2\mathbf{k}_i \cdot \mathbf{p} + p^2 - i\varepsilon)^{-1}$ . The quantity  $G_0^{(2)}(\mathbf{R})$  is given by [25]

$$G_0^{(2)}(\mathbf{R}) = (2\pi)^{-3} \exp(i\mathbf{k}_i \cdot \mathbf{R}) \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{(2kp_z - i\varepsilon)^2} p^2 \quad (9.13)$$

while

$$I^{(1)}(\mathbf{r}) = (2\pi)^{-3} \int d\mathbf{R} \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{2kp_z - i\varepsilon} U(\mathbf{r} - \mathbf{R}) \phi(\mathbf{r} - \mathbf{R}) \quad (9.14)$$

and

$$I^{(2)}(\mathbf{r}) = - (2\pi)^{-3} \int d\mathbf{R} \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{(2kp_z - i\varepsilon)^2} p^2 U(\mathbf{r} - \mathbf{R}) \phi(\mathbf{r} - \mathbf{R}). \quad (9.15)$$

Let us first examine the  $\mathbf{p}$  integral that appears in eqs. (9.12) and (9.14). Choosing Cartesian coordinates in  $\mathbf{p}$  space and denoting the components of  $\mathbf{R}$  by  $(X, Y, Z)$ , we have

$$\begin{aligned} \int d\mathbf{p} \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{2kp_z - i\varepsilon} &= \int_{-\infty}^{+\infty} dp_x \int_{-\infty}^{+\infty} dp_y \int_{-\infty}^{+\infty} dp_z \\ &\times \frac{\exp\{i(p_x X + p_y Y + p_z Z)\}}{2kp_z - i\varepsilon}. \end{aligned} \quad (9.16)$$

The integrals over  $p_x$  and  $p_y$  are easily performed, giving

$$\int dp \frac{\exp(i\mathbf{p} \cdot \mathbf{R})}{2kp_z - i\epsilon} = (2\pi)^2 \delta(X) \delta(Y) \frac{1}{2k} \int_{-\infty}^{+\infty} dp_z \frac{\exp(ip_z Z)}{p_z - i\epsilon}. \quad (9.17)$$

The integral over  $p_z$  can be done in the complex  $p_z$  plane, where the integrand has a pole at  $p_z = +i\epsilon$ . For  $Z > 0$ , we choose the integration contour as the real axis plus an infinite semi-circle  $C_1$  in the upper half plane (see Fig. 9.1). Then, applying Cauchy's theorem, we have

$$\int_{-\infty}^{+\infty} dp_z \frac{\exp(ip_z Z)}{p_z - i\epsilon} = 2\pi i, \quad (Z > 0). \quad (9.18)$$

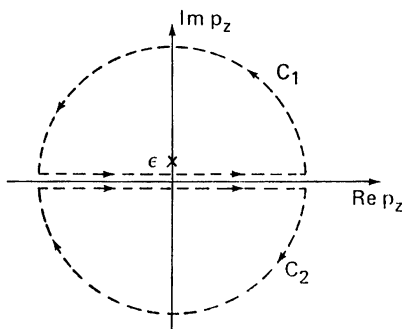


Fig. 9.1. The contours  $C_1$  and  $C_2$  used to perform the  $p_z$  integral of eq. (9.17) in the complex  $p_z$  plane. The integrand has a pole on the positive imaginary axis at  $p_z = i\epsilon$ .

For  $Z < 0$ , we close the contour by means of the infinite semi-circle  $C_2$  in the lower half-plane, thus obtaining

$$\int_{-\infty}^{+\infty} dp_z \frac{\exp(ip_z Z)}{p_z - i\epsilon} = 0, \quad (Z < 0). \quad (9.19)$$

Therefore, if we retain only the first term on the right of eq. (9.10) we have

$$G_0^{(+)}(\mathbf{R}) \simeq G_0^{(1)}(\mathbf{R}) = \begin{cases} -\frac{i}{2k} \exp(ikZ) \delta(X) \delta(Y), & Z > 0 \\ 0, & Z < 0 \end{cases} \quad (9.20)$$

or, returning to the original variables  $\mathbf{r}(x, y, z)$  and  $\mathbf{r}'(x', y', z')$ ,

$$\begin{aligned} G_0^{(+)}(\mathbf{r}, \mathbf{r}') &\simeq G_0^{(1)}(\mathbf{r}, \mathbf{r}') \\ &= \begin{cases} -\frac{i}{2k} \exp\{ik(z - z')\} \delta(x - x') \delta(y - y'), & (z - z') > 0 \\ 0, & (z - z') < 0. \end{cases} \end{aligned} \quad (9.21)$$

Introducing the step function  $\Theta(x)$  such that

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \quad (9.22)$$

we may also write eq. (9.21) as

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}') \simeq G_0^{(1)}(\mathbf{r}, \mathbf{r}') = -\frac{i}{2k} \exp\{ik(z - z')\} \times \delta(x - x')\delta(y - y')\Theta(z - z'). \quad (9.23)$$

It is obvious that the linearized propagator  $G_0^{(1)}(\mathbf{r}, \mathbf{r}')$  describes purely *forward* propagation. Using eqs. (9.17)–(9.19) in eq. (9.14) we also find that the corresponding value of the quantity  $I^{(1)}(\mathbf{r})$  is given by

$$I^{(1)}(x, y, z) = \frac{i}{2k} \int_0^\infty U(x, y, z - Z)\phi(x, y, z - Z) dZ. \quad (9.24)$$

The correction term  $I^{(2)}(\mathbf{r})$  appearing in eqs. (9.11) and (9.15) may be studied in a similar way [8]. We have already shown above that we expect this term to be small with respect to  $I^{(1)}$  when  $ka \gg 1$ . However, if we want to neglect the contribution of  $I^{(2)}$  in evaluating  $\phi(\mathbf{r})$ , we see from eq. (9.7) that it is not enough that  $|I^{(2)}|$  be small with respect to  $|I^{(1)}|$ ; it must also be small with respect to one. A careful analysis of this last condition shows that it is satisfied when  $|V_0|/E \ll 1$  [22]. We shall therefore neglect the term  $I^{(2)}$  in what follows.

Let us now come back to eq. (9.7) in which we replace  $I(\mathbf{r})$  by  $I^{(1)}(\mathbf{r})$ . The corresponding function  $\phi^{(1)}(\mathbf{r})$  satisfies the equation

$$\phi^{(1)}(x, y, z) = 1 - \frac{i}{2k} \int_0^\infty U(x, y, z - Z)\phi^{(1)}(x, y, z - Z) dZ. \quad (9.25)$$

Changing variables to

$$z' = z - Z \quad (9.26)$$

we obtain

$$\phi^{(1)}(x, y, z) = 1 - \frac{i}{2k} \int_{-\infty}^z U(x, y, z')\phi^{(1)}(x, y, z') dz' \quad (9.27)$$

and therefore

$$\phi^{(1)}(x, y, z) = \exp\left\{-\frac{i}{2k} \int_{-\infty}^z U(x, y, z') dz'\right\}. \quad (9.28)$$

Notice that  $\phi^{(1)}$  varies negligibly over distances of order  $k^{-1}$  since  $U_0/k^2$  is small. We also remark that the integral (9.28) is evaluated along a straight line parallel to  $\mathbf{k}_i$ .

Returning to the original ansatz (9.3) we deduce that the approximate scattering wave function  $\psi_E(\mathbf{r})$  which we have obtained – the *eikonal wave function* – is such that

$$\psi_E(\mathbf{r}) = (2\pi)^{-3/2} \exp\left\{i\mathbf{k}_i \cdot \mathbf{r} - \frac{i}{2k} \int_{-\infty}^z U(x, y, z') dz'\right\} \quad (9.29)$$

or, in terms of the potential  $V(\mathbf{r}) = \hbar^2 U(\mathbf{r})/2m$ ,

$$\psi_E(\mathbf{r}) = (2\pi)^{-3/2} \exp\left\{i\mathbf{k}_i \cdot \mathbf{r} - \frac{i}{\hbar v} \int_{-\infty}^z V(x, y, z') dz'\right\} \quad (9.30)$$

where  $v = \hbar k/m$  is the magnitude of the incident velocity. Thus a simple modification of the *phase* of the incident plane wave leads to the eikonal wave function.

It is worth noting that the eikonal wave function  $\psi_E(\mathbf{r})$  does not exhibit the correct asymptotic behaviour (3.27) when  $r \rightarrow \infty$ . Only in the region where the potential is non-zero does the modulating function  $\phi(\mathbf{r})$  modify the incident plane wave. This fact does not cause any difficulty since we shall simply use the integral representation (5.40) to calculate the scattering amplitude. Therefore, we need to know the scattering wave function only where the potential is non-vanishing.

Another important point concerns the *angular range of validity* of the eikonal approximation. We recall that the eikonal Green's function (9.23) only describes *forward* propagation so that the eikonal phase in eqs. (9.28)–(9.30) is obtained by performing a *straight line* integration along the direction of  $\mathbf{k}_i$ . A more accurate evaluation of the scattering wave function would in fact involve the calculation of its phase along the actual curved classical trajectory. We therefore expect that the eikonal method will be justified for *small angle* collisions, where most of the high-energy scattering occurs (see Section 8.6). However, as we shall see below, the analysis of the angular range of validity of the eikonal approximation is more complicated than simple kinematical arguments would suggest.

### 9.1.2. The eikonal scattering amplitude

Let us use the eikonal wave function (9.29) to calculate the eikonal scattering amplitude  $f_E$ . By substitution in eq. (5.40), we find that

$$f_E = -\frac{1}{4\pi} \int d\mathbf{r} \exp(-i\mathbf{k}_f \cdot \mathbf{r}) U(\mathbf{r}) \exp\left\{i\mathbf{k}_i \cdot \mathbf{r} - \frac{i}{2k} \int_{-\infty}^z U(x, y, z') dz'\right\} \quad (9.31)$$

or

$$f_E = -\frac{1}{4\pi} \int d\mathbf{r} \exp(i\Delta \cdot \mathbf{r}) U(\mathbf{r}) \exp\left\{-\frac{i}{2k} \int_{-\infty}^z U(x, y, z') dz'\right\} \quad (9.32)$$

where  $\Delta = \mathbf{k}_i - \mathbf{k}_f$  is the wave vector transfer. Now we have just noted above that the actual phase of the scattering wave function should be evaluated in the semi-classical limit along the classical path. As a partial concession to this point of view, we shall perform the  $z'$  integration in eq. (9.32) along a direction  $\hat{n}$  parallel to the bisector of the scattering angle (and therefore

perpendicular to the vector  $\Delta$ ). This is illustrated in Fig. 9.2. Furthermore, we adopt a cylindrical coordinate system and decompose the vector  $\mathbf{r}$  as

$$\mathbf{r} = \mathbf{b} + z\hat{\mathbf{n}} \quad (9.33)$$

where the  $z$  component of  $\mathbf{r}$  lies along  $\hat{\mathbf{n}}$  and  $\mathbf{b}$  is an "impact parameter" vector [26] perpendicular to  $\hat{\mathbf{n}}$ . We may therefore write eq. (9.32) as

$$f_E = -\frac{1}{4\pi} \int d^2\mathbf{b} \int_{-\infty}^{+\infty} dz \exp(i\Delta \cdot \mathbf{b}) U(\mathbf{b}, z) \times \exp\left\{-\frac{i}{2k} \int_{-\infty}^z U(\mathbf{b}, z') dz'\right\}. \quad (9.34)$$

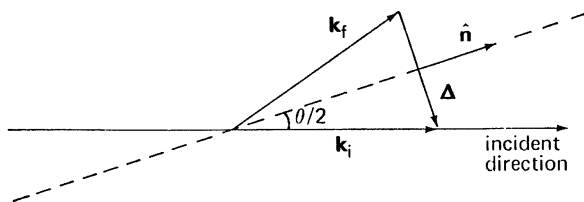


Fig. 9.2. Illustration of the vectors involved in eqs. (9.32) and (9.33).

It is worth noting that eq. (9.34) may also be derived by performing the  $z'$  integration in eq. (9.32) along the original direction  $\hat{\mathbf{k}}_i$  and then using the fact that for small scattering angles the vector  $\Delta$  is nearly perpendicular to  $\mathbf{k}_i$ . In this case the cylindrical coordinate system in  $\mathbf{r}$  space is chosen in such a way that

$$\mathbf{r} = \mathbf{b} + z\hat{\mathbf{k}}_i \quad (9.35)$$

and we have

$$\Delta \cdot \mathbf{r} = \Delta \cdot (\mathbf{b} + z\hat{\mathbf{k}}_i) = \Delta \cdot \mathbf{b} + kz(1 - \cos \theta) \simeq \Delta \cdot \mathbf{b} \quad (9.36)$$

where terms of order  $\theta^2 kz \lesssim \theta^2 ka$  have been neglected. Therefore, in this coordinate system, a qualitative angular validity criterion is given by  $\theta \ll (ka)^{-1/2}$ . It is not unreasonable to expect that the choice of coordinate system (9.33) will lead to an improved (larger) angular domain of validity of the eikonal approximation [3]. That this is indeed the case will be illustrated below.

The integration over the  $z$  variable in eq. (9.34) is now straightforward. We find that the eikonal scattering amplitude is given by

$$f_E = \frac{k}{2\pi i} \int d^2\mathbf{b} \exp(i\Delta \cdot \mathbf{b}) [\exp\{i\chi(k, \mathbf{b})\} - 1] \quad (9.37)$$

where the quantity

$$\chi(k, \mathbf{b}) = -\frac{1}{2k} \int_{-\infty}^{+\infty} U(\mathbf{b}, z) dz \quad (9.38)$$

is called the *eikonal phase shift function*. In writing eq. (9.37) we shall agree that the cylindrical coordinate system (9.33) has been chosen with  $\hat{n}$  perpendicular to  $\Delta$ .

For potentials which possess cylindrical symmetry, we can simplify eq. (9.37) by noting that the ordinary Bessel function  $J_0$  is given by

$$J_0(x) = (2\pi)^{-1} \int_0^{2\pi} d\phi \exp(ix \cos \phi). \quad (9.39)$$

If we choose  $\Delta$  as the  $x$ -axis in the plane perpendicular to  $\hat{n}$  (so that the polar angle  $\phi$  of  $\mathbf{b}$  is measured from  $\Delta$ ) we have  $\Delta \cdot \mathbf{b} = \Delta b \cos \phi$  and eq. (9.37) reduces with the help of (9.39) to

$$f_E = \frac{k}{i} \int_0^\infty db \, b J_0(\Delta b) [\exp\{i\chi(k, b)\} - 1] \quad (9.40)$$

where  $\Delta = 2k \sin \frac{1}{2}\theta$  and the phase shift function  $\chi$  now depends only on  $k$  and  $b$ .

It is a simple matter to establish the relationship between the eikonal scattering amplitude (9.40) and the amplitude (4.63) which appears in the method of partial waves. Indeed, let us first use the formula

$$P_l(\cos \theta) \simeq J_0[(l + \frac{1}{2})\theta] \quad (9.41)$$

valid [27] for  $l \gg 1$  and  $l\theta = \mathcal{O}(1)$ . Eq. (4.63) then becomes

$$f(\theta) \simeq \frac{1}{ik} \sum_{l=0}^{\infty} (l + \frac{1}{2}) J_0[(l + \frac{1}{2})\theta] [\exp(2i\delta_l) - 1]. \quad (9.42)$$

Since the number of important partial waves is large at high energies, we may replace the sum over  $l$  by an integral over the impact parameter  $b$ . Using the fact that

$$b \simeq \sqrt{l(l+1)}/k = (l + \frac{1}{2} + \dots)/k \quad (9.43)$$

we may then write

$$f(\theta) = \frac{k}{i} \int_0^\infty db \, b J_0(2kb \sin \frac{1}{2}\theta) [\exp\{2i\delta(k, b)\} - 1] \quad (9.44)$$

where

$$\delta(k, b) \equiv \delta_l(k), \quad l + \frac{1}{2} \simeq kb \quad (9.45)$$

and we have replaced  $kb\theta$  by  $2kb \sin \frac{1}{2}\theta$  in the argument of the Bessel function  $J_0$ . This replacement is justified since we are dealing here with *small angle* scattering where the approximate formula (9.41) is valid. The formula (9.44) then reduces to (9.40), with

$$\delta(k, b) = \frac{1}{2}\chi(k, b) = -\frac{1}{4k} \int_{-\infty}^{+\infty} U(b, z) dz. \quad (9.46)$$

We shall now verify that the eikonal approximation satisfies the optical theorem in the limit of high energies. Indeed, let us tentatively write the total (complete) cross section in the eikonal approximation as

$$\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im } f_E(\theta = 0) = 4\pi \int_0^\infty db \, b [1 - \exp(-\text{Im } \chi) \cos(\text{Re } \chi)] \quad (9.47)$$

where we have considered a complex (optical) potential  $U$  having azimuthal symmetry and we have written

$$\chi(k, b) = \text{Re } \chi(k, b) + i \text{Im } \chi(k, b). \quad (9.48)$$

Now the total *elastic* cross section is simply

$$\begin{aligned} \sigma_{\text{tot}}^{\text{el}} &= \int d\Omega |f_E|^2 \\ &= k^2 \int_0^\infty db \, b \int_0^\infty db' \, b' [\exp\{i\chi(k, b)\} - 1] [\exp\{-i\chi^*(k, b')\} - 1] \\ &\quad \times \int d\Omega J_0(2kb \sin \tfrac{1}{2}\theta) J_0(2kb' \sin \tfrac{1}{2}\theta). \end{aligned} \quad (9.49)$$

Performing the azimuthal integration and changing the integration variable from  $\theta$  to  $\Delta = 2k \sin \tfrac{1}{2}\theta$  we find that

$$\begin{aligned} \sigma_{\text{tot}}^{\text{el}} &= 2\pi \int_0^\infty db \, b \int_0^\infty db' \, b' [\exp\{i\chi(k, b)\} - 1] [\exp\{-i\chi^*(k, b')\} - 1] \\ &\quad \times \int_0^{2k} d\Delta \, \Delta J_0(\Delta b) J_0(\Delta b'). \end{aligned} \quad (9.50)$$

At high energies, where the eikonal approximation is valid we may extend the upper limit of the  $\Delta$ -integral to infinity. Then, using the completeness relation for the Bessel function  $J_0$ , i.e.

$$\int_0^\infty J_0(\Delta b) J_0(\Delta b') \Delta \, d\Delta = \frac{1}{b} \delta(b - b') \quad (9.51)$$

we obtain a simple approximate expression for  $\sigma_{\text{tot}}^{\text{el}}$ , namely

$$\begin{aligned} \sigma_{\text{tot}}^{\text{el}} &= 4\pi \int_0^\infty db \, b [1 - \exp(-\text{Im } \chi) \cos(\text{Re } \chi)] \\ &\quad - 2\pi \int_0^\infty db \, b [1 - \exp(-2 \text{Im } \chi)]. \end{aligned} \quad (9.52)$$

We first note that when the potential  $U$  is real, so that  $\text{Im } \chi = 0$ , this expression agrees with eq. (9.47). When the potential is complex we find by comparing eqs. (9.47) and (9.52) that the total cross section for non-elastic processes  $\sigma_{\text{tot}}^{\text{r}}$  is given by

$$\sigma_{\text{tot}}^{\text{r}} = \sigma_{\text{tot}} - \sigma_{\text{tot}}^{\text{el}} = 2\pi \int_0^\infty db \, b [1 - \exp(-2 \text{Im } \chi)]. \quad (9.53)$$

This is a very reasonable result. Indeed, the intensity of a wave having unit amplitude and corresponding to the impact parameter  $b$  is simply



$\exp(-2 \operatorname{Im} \chi)$  after it has penetrated through the region where the potential acts. Hence the quantity  $1 - \exp(-2 \operatorname{Im} \chi)$  yields the absorption due to the area  $2\pi b db$  contained between two circles of radius  $b$  and  $(b + db)$ , respectively.

We may easily generalize these considerations to the case where there is no azimuthal symmetry. Using eq. (9.37), we then have

$$\sigma_{\text{tot}} = \frac{4\pi}{k} \operatorname{Im} f_E(\theta = 0) = 2 \int d^2 b [1 - \exp(-\operatorname{Im} \chi) \cos(\operatorname{Re} \chi)] \quad (9.54)$$

where the phase shift function is given by eq. (9.38).

The total *elastic* cross section is now obtained from the scattering amplitude (9.37) by writing

$$\begin{aligned} \sigma_{\text{tot}}^{\text{el}} &= \int d\Omega |f_E|^2 \\ &= \left(\frac{k}{2\pi}\right)^2 \int d\Omega \int d^2 b \int d^2 b' \exp\{i\mathbf{A} \cdot (\mathbf{b} - \mathbf{b}')\} \\ &\quad \times [\exp\{i\chi(k, \mathbf{b})\} - 1] [\exp\{-i\chi^*(k, \mathbf{b}')\} - 1]. \end{aligned} \quad (9.55)$$

Since the scattering is sharply concentrated near the forward direction at high energies, we may replace the integration over  $d\Omega$  by an integration over the vectors  $\mathbf{A}$  lying in a plane perpendicular to  $\mathbf{k}_i$ . We may then write approximately

$$\begin{aligned} \sigma_{\text{tot}}^{\text{el}} &= (2\pi)^{-2} \int d^2 A \int d^2 b \int d^2 b' \exp\{i\mathbf{A} \cdot (\mathbf{b} - \mathbf{b}')\} \\ &\quad \times [\exp\{i\chi(k, \mathbf{b})\} - 1] [\exp\{-i\chi^*(k, \mathbf{b}')\} - 1] \end{aligned} \quad (9.56)$$

and since

$$\int \exp\{i\mathbf{A} \cdot (\mathbf{b} - \mathbf{b}')\} d^2 A = (2\pi)^2 \delta^{(2)}(\mathbf{b} - \mathbf{b}') \quad (9.57)$$

we find that

$$\sigma_{\text{tot}}^{\text{el}} = \int |\exp(i\chi) - 1|^2 d^2 b. \quad (9.58)$$

We note that when there is no absorption so that  $\chi$  is real, eq. (9.58) agrees with the expression (9.54) of the total (complete) cross section. We also find by analogy with eq. (9.53) that in the presence of absorption the total cross section for non-elastic processes is now given by

$$\sigma_{\text{tot}}^{\text{r}} = \sigma_{\text{tot}} - \sigma_{\text{tot}}^{\text{el}} = \int d^2 b [1 - \exp(-2 \operatorname{Im} \chi)]. \quad (9.59)$$

Of course the formulae (9.54), (9.58) and (9.59) reduce respectively to eqs. (9.47), (9.52) and (9.53) when the phase shift function has azimuthal symmetry.

Let us illustrate the foregoing discussion on a simple example. We consider the scattering by a complex square well

$$U(r) = \begin{cases} -U_0, & r < a \\ 0, & r > a \end{cases} \quad (9.60)$$

with

$$U_0 = U_R + iU_I \quad (U_R, U_I > 0). \quad (9.61)$$

Then, according to eq. (9.40),

$$f_E = \frac{k}{i} \int_0^\infty db \, b J_0(2kb \sin \tfrac{1}{2}\theta) [\exp\{i\chi(k, b)\} - 1] \quad (9.62)$$

with

$$\chi(b, k) = \begin{cases} \frac{U_0}{k} \sqrt{a^2 - b^2}, & \text{for } 0 \leq b < a \\ 0, & \text{for } b > a. \end{cases} \quad (9.63)$$

Therefore,

$$f_E = \frac{k}{i} \int_0^a db \, b J_0(2kb \sin \tfrac{1}{2}\theta) \left[ \exp\left\{i \frac{U_0}{k} \sqrt{a^2 - b^2}\right\} - 1 \right]. \quad (9.64)$$

We note that

$$|e^{i\chi}|^2 = \exp(-2 \operatorname{Im} \chi) = \exp\left\{-\frac{U_I}{k} 2\sqrt{a^2 - b^2}\right\}, \quad 0 \leq b < a. \quad (9.65)$$

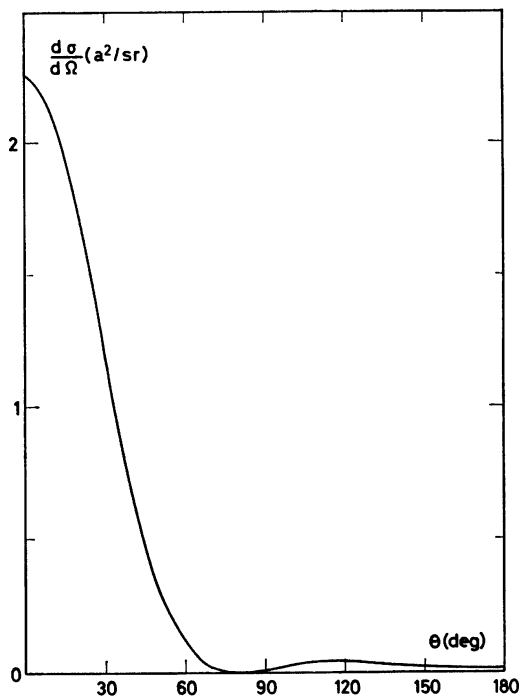


Fig. 9.3. Illustration of the differential cross section (9.69) of the text. Here  $ka = 3$ .

Since  $D = 2\sqrt{a^2 - b^2}$  is the distance travelled through the interaction region and corresponding to the "impact parameter"  $b$ , we can interpret the quantity  $\Lambda = k/U_1$  as the *mean free path* through the potential. For very small mean free paths, corresponding to strong absorption, so that

$$k/U_1 \ll a \quad \text{or} \quad U_1 a/k \gg 1 \quad (9.66)$$

we may neglect the exponential in eq. (9.64) and write

$$f_E = ik \int_0^a db \, b J_0(2kb \sin \frac{1}{2}\theta). \quad (9.67)$$

This last integral is easily performed. One has

$$f_E = ika^2 \frac{J_1(2ka \sin \frac{1}{2}\theta)}{2ka \sin \frac{1}{2}\theta} \quad (9.68)$$

so that the corresponding differential cross section reads

$$\left(\frac{d\sigma}{d\Omega}\right)_E = a^2(ka)^2 \left[ \frac{J_1(2ka \sin \frac{1}{2}\theta)}{2ka \sin \frac{1}{2}\theta} \right]^2. \quad (9.69)$$

This is a well known result in optics [see e.g. 28] where it characterizes the Fraunhofer diffraction scattering by a black sphere. The angular distribution corresponding to eq. (9.69) is illustrated in Fig. 9.3 for the case  $ka = 3$ . We note from eq. (9.69) that when  $ka \gg 1$  there is a large forward peak having a width of order  $1/ka$ .

### 9.1.3. The eikonal approximation and the Born series

Let us return to the eikonal scattering amplitude (9.37). By expanding the quantity  $\exp(i\chi)$  in powers of  $\chi$  – and hence in powers of the potential – we define the *eikonal multiple scattering series*

$$f_E = \sum_{n=1}^{\infty} \tilde{f}_{En} \quad (9.70)$$

where

$$\tilde{f}_{En} = \frac{k}{2\pi i} \frac{i^n}{n!} \int d^2\mathbf{b} \exp(i\mathbf{A} \cdot \mathbf{b}) [\chi(k, \mathbf{b})]^n. \quad (9.71)$$

We note that if the summation and integration may be interchanged the series (9.70) always converges since  $\exp(z)$  is an entire function of  $z$ . By analogy with our study of the Born series we also define the quantity

$$f_{En} = \sum_{j=1}^n \tilde{f}_{Ej}. \quad (9.72)$$

We shall now examine more closely the quantity  $\tilde{f}_{E1} = f_{E1}$ . Using eqs. (9.38) and (9.71), we have

$$f_{E1} = -\frac{1}{4\pi} \int d^2\mathbf{b} \int_{-\infty}^{+\infty} dz \exp(i\mathbf{A} \cdot \mathbf{b}) U(\mathbf{b}, z). \quad (9.73)$$

With the choice of cylindrical coordinate system (9.33) such that the vector  $\Delta$  entirely lies in the plane of "impact parameters"  $\mathbf{b}$ , we have  $\Delta \cdot \mathbf{b} = \Delta \cdot \mathbf{r}$  and therefore

$$f_{E1} = -\frac{1}{4\pi} \int d\mathbf{r} \exp(i\Delta \cdot \mathbf{r}) U(\mathbf{r}) \quad (9.74)$$

or [see eq. (8.30)]

$$f_{E1} = f_{B1} \quad (9.75)$$

where  $f_{B1}$  is the first Born approximation to the scattering amplitude.

This is an important relation, valid for all potentials (subject to the condition that the above quantities be defined) and all scattering angles. We note that if the  $z$  integration in eq. (9.38) had been performed along the direction  $\hat{\mathbf{k}}_1$ , using the coordinate system (9.35), we would only have approximately  $\Delta \cdot \mathbf{b} \simeq \Delta \cdot \mathbf{r}$  for small  $\Delta$ 's and the relation (9.75) would only hold at *small angles*. Since we know that the Born series converges at sufficiently high energies for non-relativistic potential scattering (see Section 8.4) it is very desirable to secure the relation (9.75) at *all angles* as our "starting point" of the eikonal multiple scattering series. Therefore the result (9.75) lends additional support to the semi-classical argument made after eq. (9.32) about the choice of the direction  $\hat{\mathbf{n}}$  along the bisector of the scattering angle. It actually goes beyond this argument since eq. (9.75) holds for *all* values of  $\theta$ , including those large scattering angles for which the simple reasoning following eq. (9.32) is no more valid. Thus we shall continue in what follows to choose the direction  $\hat{\mathbf{n}}$  perpendicular to  $\Delta$ .

We now want to compare the *higher order* terms of the eikonal and Born series [29]. We shall simplify our discussion by considering only *central, real* potentials. In this case the quantities  $\tilde{f}_{En}$  reduce to

$$\tilde{f}_{En} = -\frac{i^{n+1}k}{n!} \int_0^\infty J_0(\Delta b) [\chi(k, b)]^n b db. \quad (9.76)$$

We note that these expressions are alternatively real and imaginary, a fact which plays an important role in the discussion given below.

Let us consider the second terms  $\tilde{f}_{E2}$  and  $\tilde{f}_{B2}$  of the eikonal series (9.70) and the Born series (8.18), respectively. Since  $\text{Re } \tilde{f}_{E2} = 0$  while in general  $\text{Re } \tilde{f}_{B2} \neq 0$ , there is no analogue of eq. (9.75) for  $\text{Re } \tilde{f}_{B2}$  and  $\text{Re } \tilde{f}_{E2}$ . We shall return to this point below in our discussion of the relative merits of the second Born and eikonal approximations. For the moment, we focus our attention on  $\text{Im } \tilde{f}_{B2}$  and  $\text{Im } \tilde{f}_{E2}$  and consider first a simple particular case, i.e. a Yukawa potential of the form [30]

$$U(r) = -U_0 e^{-ar}/r \quad (9.77)$$

for which the quantity  $\tilde{f}_{B2}(k, \Delta)$  is given by eq. (8.99). On the other hand, for the same interaction (9.77) the eikonal phase shift function is given by [see e.g. 31]

$$\chi(k, b) = \frac{U_0}{k} K_0(\alpha b) \quad (9.78)$$

where  $K_0$  is a modified Bessel function of order zero. Therefore, one has from eq. (9.76)

$$\tilde{f}_{E2} = i \frac{U_0^2}{2k} \int_0^\infty J_0(\Delta b) [K_0(\alpha b)]^2 b \, db. \quad (9.79)$$

This integral may be performed, with the result [see e.g. 32]

$$\tilde{f}_{E2} = i \frac{U_0^2}{2\Delta[4k^2\alpha^2 + k^2\Delta^2]^{1/2}} \log \frac{(4k^2\alpha^2 + k^2\Delta^2)^{1/2} + k\Delta}{(4k^2\alpha^2 + k^2\Delta^2)^{1/2} - k\Delta}. \quad (9.80)$$

Let us now return to eq. (8.99) which gives the second Born term  $\tilde{f}_{B2}(k, \Delta)$  for the Yukawa potential (9.77). For *large*  $k$  we note that the leading term of  $\tilde{f}_{B2}$  is purely imaginary [see eqs. (8.100)–(8.101)] and such that

$$\tilde{f}_{B2}(k, \Delta) = A_{B2}(\Delta)/k + \dots \quad (9.81)$$

where the quantity  $A_{B2}(\Delta)$  depends *only* on  $\Delta$  and we have neglected terms of higher order in  $k^{-1}$  [33]. On the other hand, we may write eq. (9.80) in the form

$$\tilde{f}_{E2}(k, \Delta) = A_{E2}(\Delta)/k \quad (9.82)$$

and upon comparison of eqs. (8.99) and (9.80) we see that

$$A_{E2}(\Delta) = A_{B2}(\Delta) \quad (9.83)$$

for *all wave vector transfers*  $\Delta$ . Thus, when  $k$  is large enough so that eq. (9.81) holds, one has

$$\text{Im } \tilde{f}_{E2}(k, \Delta) = \text{Im } \tilde{f}_{B2}(k, \Delta) \quad (9.84)$$

for all values of  $\Delta$ .

It is a simple matter to generalize eq. (9.83) to an arbitrary superposition of Yukawa potentials of the form (8.105) namely

$$U(r) = -U_0 \int_{v_0 > 0}^\infty \rho(v) \frac{e^{-vr}}{r} \, dv. \quad (9.85)$$

Indeed, the quantity  $\tilde{f}_{E2}$  is now given by

$$\tilde{f}_{E2} = \frac{iU_0^2}{2k} \int_{v_0}^\infty d\mu \, \rho(\mu) \int_{v_0}^\infty dv \, \rho(v) \int_0^\infty J_0(\Delta b) K_0(\mu b) K_0(vb) b \, db. \quad (9.86)$$

The integral on the variable  $b$  may again be done [see e.g. 34] and yields

$$\tilde{f}_{E2} = \frac{iU_0^2}{4k} \int_{v_0}^\infty d\mu \int_{v_0}^\infty dv \, \rho(\mu) \rho(v) \frac{1}{\mu v \sqrt{u^2 - 1}} \log[u + \sqrt{u^2 - 1}] \quad (9.87)$$

with

$$u = (\mu^2 + \nu^2 + \Delta^2)/2\mu\nu. \quad (9.88)$$

Hence we see that eq. (9.83) follows by comparing eq. (9.87) with the asymptotic expression (8.113) of  $\bar{f}_{B2}$ , valid for high wave numbers  $k$ .

Since eq. (9.84) deals with the region of "large"  $k$ , it is interesting to investigate when this asymptotic behaviour actually sets in. A simple look at eqs. (8.99) and (9.80) shows that  $ka$  (with  $a = \alpha^{-1}$ ) does not have to be much greater than one for the asymptotic equation (9.84) to hold fairly accurately in the case of the simple Yukawa potential (9.77). This is illustrated

TABLE 9.1

Comparison of  $\text{Im } \bar{f}_{B2}/U_0^2$  and  $\text{Im } \bar{f}_{E2}/U_0^2$  for a Yukawa potential  $U(r) = -U_0 e^{-r}/r$  and for various values of the scattering angle  $\theta$  and the wave number  $k$  (taken from ref. [22]). The unit of length is the "range"  $a = \alpha^{-1}$  of the potential. The numbers in parentheses indicate powers of 10.

$k$	$\theta$ (degrees)	$\text{Im } \bar{f}_{B2}/U_0^2$	$\text{Im } \bar{f}_{E2}/U_0^2$
1	0	2.00 (−1)	2.50 (−1)
	90	1.59 (−1)	1.90 (−1)
	180	1.34 (−1)	1.56 (−1)
2	0	1.18 (−1)	1.25 (−1)
	90	5.66 (−2)	5.85 (−2)
	180	3.94 (−2)	4.04 (−2)
3	0	8.11 (−2)	8.33 (−2)
	90	2.48 (−2)	2.51 (−2)
	180	1.58 (−2)	1.60 (−2)
5	0	4.95 (−2)	5.00 (−2)
	90	7.58 (−3)	7.60 (−3)
	180	4.52 (−3)	4.54 (−3)
10	0	2.49 (−2)	2.50 (−2)
	90	1.31 (−3)	1.31 (−3)
	180	7.46 (−4)	7.46 (−4)

in Table 9.1, where  $\text{Im } \bar{f}_{B2}/U_0^2$  and  $\text{Im } \bar{f}_{E2}/U_0^2$  are compared for the potential (9.77) for several values of  $k$  and of the scattering angle  $\theta$ . We note that the agreement between  $\text{Im } \bar{f}_{B2}/U_0^2$  and  $\text{Im } \bar{f}_{E2}/U_0^2$  is always poorest in the forward direction [35]. A similar comparison is made in Table 9.2 for the superposition of two Yukawa potentials considered in Section 8.6, namely

$$U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r \quad (9.89)$$

where the "range" of the first Yukawa potential is the unit of length. The conclusions are essentially the same as for the simple Yukawa potential (9.77) although the angle at which the agreement is poorest now depends on the wave number.

We have examined so far the quantities  $\bar{f}_{B2}$  and  $\bar{f}_{E2}$  for Yukawa-type potentials. It may also be proved that eq. (9.84) holds for large  $k$  and *all* momentum transfers in the case of exponential potentials of the form  $U(r) = -U_0 \exp(-\alpha r)$ . On the contrary, for various other interactions it may be shown that the relation (9.84) only holds for large  $k$  and *small* momentum transfers [36].

TABLE 9.2

Comparison of  $\text{Im} \bar{f}_{B2}/U_0^2$  and  $\text{Im} \bar{f}_{E2}/U_0^2$  for a superposition of two Yukawa potentials  $U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r$  and for various values of the scattering angle  $\theta$  and the wave number  $k$  (taken from ref. [22]). The unit of length is the "range" of the first Yukawa potential

$k$	$\theta$ (degrees)	$\text{Im} \bar{f}_{B2}/U_0^2$	$\text{Im} \bar{f}_{E2}/U_0^2$
1	0	6.77 (-2)	6.92 (-2)
	90	4.10 (-2)	3.63 (-2)
	180	2.68 (-2)	2.15 (-2)
2	0	3.46 (-2)	3.46 (-2)
	90	4.86 (-3)	4.56 (-3)
	180	1.07 (-3)	1.09 (-3)
3	0	2.30 (-2)	2.31 (-2)
	90	4.73 (-4)	5.10 (-4)
	180	-1.67 (-4)	-1.13 (-4)
5	0	1.38 (-2)	1.38 (-2)
	90	-1.15 (-4)	-1.04 (-4)
	180	-9.29 (-5)	-8.65 (-5)
10	0	6.92 (-3)	6.92 (-3)
	90	-2.47 (-5)	-2.43 (-5)
	180	-1.22 (-5)	-1.20 (-5)

The comparison of the terms  $\bar{f}_{Bn}$  and  $\bar{f}_{En}$  for  $n \geq 3$  and large  $k$  is a difficult problem which we shall not treat in detail here. For *Yukawa-type potentials* the generalization of eq. (9.81) reads [21, 22]

$$\bar{f}_{Bn}(k, \Delta) = \frac{A_{Bn}(\Delta)}{k^{n-1}} + \mathcal{O}(k^{-n}) \quad (9.90)$$

where the function  $A_{Bn}(\Delta)$  only depends on  $\Delta$ . Then, defining the quantity  $A_{En}(\Delta)$  by the relation [see eq. (9.82)]

$$\bar{f}_{En}(k, \Delta) = A_{En}(\Delta)/k^{n-1} \quad (9.91)$$

one has [37]

$$A_{Bn}(\Delta) = A_{En}(\Delta) \quad (9.92)$$

for all  $n$  and all values of the momentum transfer. Remembering that the quantities  $\bar{f}_{En}$  are alternatively real and purely imaginary, we see that for

large enough  $k$  (and Yukawa-type potentials) the relations (9.90)–(9.92) imply that

$$\bar{f}_{E3}(k, \Delta) = \operatorname{Re} \bar{f}_{B3}(k, \Delta), \quad (9.93a)$$

$$\operatorname{Im} \bar{f}_{E4}(k, \Delta) = \operatorname{Im} \bar{f}_{B4}(k, \Delta), \quad (9.93b)$$

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$$\bar{f}_{En}(k, \Delta) = \operatorname{Re} \bar{f}_{Bn}(k, \Delta), \quad n \text{ odd} \quad (9.93c)$$

$$\operatorname{Im} \bar{f}_{En}(k, \Delta) = \operatorname{Im} \bar{f}_{Bn}(k, \Delta), \quad n \text{ even.} \quad (9.93d)$$

As an illustration of eq. (9.93a), we display in Table 9.3 the comparison of  $\operatorname{Re} \bar{f}_{B3}/U_0^3$  with  $\bar{f}_{E3}/U_0^3$  for the simple Yukawa potential (9.77) and a wave number  $k = 5$ . The agreement between the two quantities is seen to be excellent for all values of the scattering angle. A similar comparison is shown in Table 9.4 for the “double Yukawa” potential (9.89) with essentially the same conclusions.

TABLE 9.3

Comparison of  $\operatorname{Re} \bar{f}_{B3}/U_0^3$  with  $\bar{f}_{E3}/U_0^3$  for a Yukawa potential  $U(r) = -U_0 e^{-r}/r$  and a wave member  $k = 5$  (taken from ref. [22]).

The unit of length is the “range”  $a = \alpha^{-1}$  of the potential

$\theta$ (degrees)	$\operatorname{Re} \bar{f}_{B3}/U_0^3$	$\bar{f}_{E3}/U_0^3$
0	−3.84 (−3)	−3.91 (−3)
30	−3.01 (−3)	−3.02 (−3)
60	−2.05 (−3)	−2.04 (−3)
90	−1.52 (−3)	−1.51 (−3)
120	−1.24 (−3)	−1.23 (−3)
150	−1.10 (−3)	−1.09 (−3)
180	−1.06 (−3)	−1.05 (−3)

Restricting ourselves to Yukawa-type potentials, we shall now analyze some of the consequences of our comparison between the eikonal and the Born multiple scattering series. We first consider the *weak coupling* case such that

$$|V_0|a/\hbar v = |U_0|a/2k \ll 1. \quad (9.94)$$

Furthermore, we impose the conditions of validity of the eikonal approximation, namely

$$ka \gg 1 \quad (9.95)$$

and

$$|V_0|/E = |U_0|/k^2 \ll 1. \quad (9.96)$$



TABLE 9.4

Comparison of  $\text{Re } \bar{f}_{B3}/U_0^3$  with  $\bar{f}_{E3}/U_0^3$  for a superposition of two Yukawa potentials  $U(r) = -U_0(e^{-r} - 1.125 e^{-2r})/r$ . The wave number is  $k = 5$  (taken from ref. [22]). The unit of length is the "range" of the first Yukawa potential

$\theta$ (degrees)	$\text{Re } \bar{f}_{B3}/U_0^3$	$\bar{f}_{E3}/U_0^3$
0	-2.79 (-4)	-2.87 (-4)
30	-9.41 (-5)	-9.31 (-5)
60	-4.52 (-6)	-6.52 (-6)
90	5.78 (-6)	4.16 (-6)
120	5.67 (-6)	4.67 (-6)
150	4.95 (-6)	4.27 (-6)
180	4.84 (-6)	4.10 (-6)

TABLE 9.5

The real part of the scattering amplitude for a superposition of two Yukawa potentials  $U(r) = -(e^{-r} - 1.125 e^{-2r})/r$  and an incident wave number  $k = 5$  (taken from ref. [22]).

$\theta$ (degrees)	$f_{B1}$	$f_{B2}$	$f_E$	$f_E + \bar{f}_{B2}$	$f$
0	7.188(-1)	7.194 (-1)	7.185 (-1)	7.191 (-1)	7.191 (-1)
30	2.474 (-2)	2.453 (-2)	2.465 (-2)	2.444 (-2)	2.444 (-2)
60	-3.316 (-4)	-3.976 (-4)	-3.381 (-4)	-4.041 (-4)	-4.021 (-4)
90	-1.225 (-3)	-1.235 (-3)	-1.221 (-3)	-1.231 (-3)	-1.229 (-3)
120	-1.083 (-3)	-1.078 (-3)	-1.078 (-3)	-1.074 (-3)	-1.073 (-3)
150	-9.577 (-4)	-9.501 (-4)	-9.534 (-4)	-9.459 (-4)	-9.452 (-4)
180	-9.163 (-4)	-9.081 (-4)	-9.122 (-4)	-9.039 (-4)	-9.032 (-4)

TABLE 9.6

The real part of the scattering amplitude for a superposition of two Yukawa potentials  $U(r) = -3(e^{-r} - 1.125 e^{-2r})/r$  and an incident wave number  $k = 5$  (taken from ref. [22]).

$\theta$ (degrees)	$f_{B1}$	$f_{B2}$	$f_E$	$f_E + \bar{f}_{B2}$	$f$
0	2.156	2.162	2.149	2.154	2.154
30	7.422 (-2)	7.236 (-2)	7.172 (-2)	6.986 (-2)	6.986 (-2)
60	-9.947 (-4)	-1.589 (-3)	-1.169 (-3)	-1.763 (-3)	-1.689 (-3)
90	-3.676 (-3)	-3.761 (-3)	-3.565 (-3)	-3.649 (-3)	-3.604 (-3)
120	-3.248 (-3)	-3.210 (-3)	-3.123 (-3)	-3.085 (-3)	-3.062 (-3)
150	-2.873 (-3)	-2.805 (-3)	-2.758 (-3)	-2.690 (-3)	-2.677 (-3)
180	-2.749 (-3)	-2.675 (-3)	-2.639 (-3)	-2.565 (-3)	-2.553 (-3)

In this case the Born series converges and we may use the asymptotic results (8.100), (8.101) and (9.90) to write the *exact scattering amplitude* for fixed  $\Delta$  and large  $k$  as

$$f(k, \Delta) = f_{B1}(\Delta) + \underbrace{\left[ \frac{A(\Delta)}{k^2} + i \frac{B(\Delta)}{k} \right]}_{\tilde{f}_{B2}} + \underbrace{\frac{C(\Delta)}{k^2}}_{\tilde{f}_{B3}} + \mathcal{O}(k^{-3}). \quad (9.97)$$

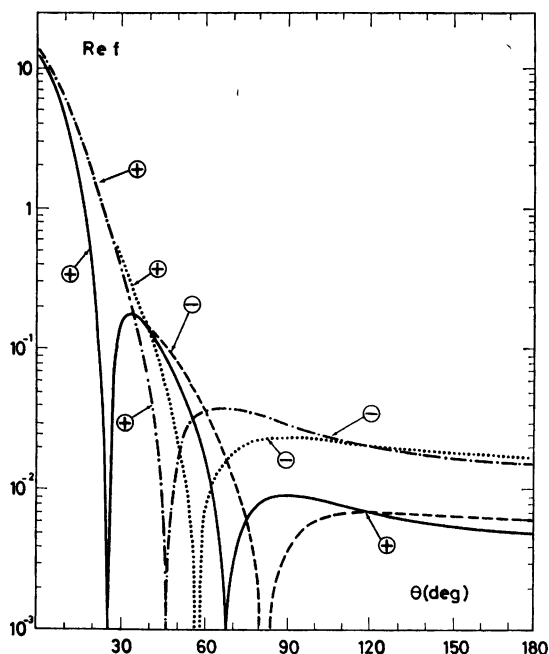


Fig. 9.4. The real part of the scattering amplitude for a superposition of two Yukawa potentials of the form (9.89), with  $U_0 = 20$  and  $k = 5$ . The solid curve shows the exact result, the dashed curve gives the eikonal result, the dotted curve represents the first Born approximation and the dash-dotted curve gives the second Born approximation. Since a logarithmic scale is used we have indicated the sign of the various quantities (taken from ref. [22]).

We have used here for convenience the functions  $A(\Delta)$  and  $B(\Delta)$  introduced respectively in eqs. (8.100) and (8.101), with  $A_{B2}(\Delta) = iB(\Delta)$  [33]. Furthermore, we have written  $C(\Delta) = A_{B3}(\Delta)$ . On the other hand, the relations (9.75), (9.91) and (9.92) imply that the eikonal scattering amplitude is given by

$$f_E(k, \Delta) = f_{B1}(\Delta) + i \frac{B(\Delta)}{k} + \frac{C(\Delta)}{k^2} + \mathcal{O}(k^{-3}). \quad (9.98)$$

$\underbrace{\hspace{1.5cm}}_{\tilde{f}_{E2}} \quad \underbrace{\hspace{1.5cm}}_{\tilde{f}_{E3}}$

Upon comparison of eqs. (9.97) and (9.98), we see that neither  $f_{B2} = f_{B1} + \bar{f}_{B2}$  nor  $f_E$  are correct to order  $k^{-2}$ . Indeed,  $f_{B2}$  lacks the term  $C(\Delta)/k^2$  (as we have already pointed out in Section 8.6) while the real term  $A(\Delta)/k^2$  is not present in  $f_E$ . Since  $A(\Delta)$  – arising from  $\bar{f}_{B2}$  – is proportional to  $U_0^2$ , while  $C(\Delta)$  – coming from  $\bar{f}_{B3}$  – is proportional to  $U_0^3$ , it is obvious that when  $U_0$  is sufficiently small the second Born amplitude  $f_{B2}$  is closer to the exact result than  $f_E$ . This is illustrated in Table 9.5 where the quantities  $f_{B1}$ ,  $\text{Re } f_{B2}$ ,  $\text{Re } f_E$ ,  $\text{Re}(f_E + \bar{f}_{B2})$  and the exact result  $\text{Re } f$  are shown for a potential of the form (9.89) with  $U_0 = 1$  and  $k = 5$  (the range  $a$  of the first Yukawa potential

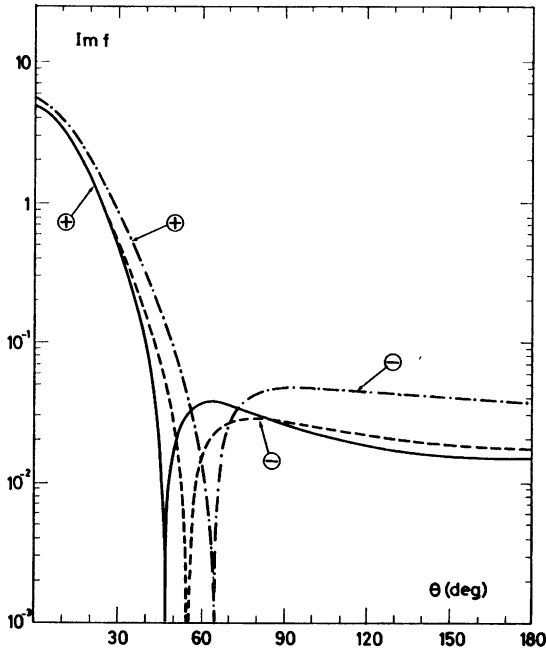


Fig. 9.5. The imaginary part of the scattering amplitude for a superposition of two Yukawa potentials of the form (9.89) with  $U_0 = 20$  and  $k = 5$ . The solid curve shows the exact result, the dashed curve gives the eikonal result and the dash-dotted curve represents the second Born approximation (taken from ref. [22]).

is the unit of length). We see from Table 9.5 that if we add to the eikonal amplitude the missing term  $\text{Re } \bar{f}_{B2}$  the improvement is spectacular. We also note from eqs. (9.97) and (9.98) that for large  $k$  and small  $|U_0|$  the *differential cross section* is given more accurately by the second Born approximation than by the eikonal method.

Let us now increase the value of  $|U_0|$ , so that we enter in the region of “*intermediate coupling*” such that

$$|V_0|a/\hbar v = |U_0|a/2k \simeq 1. \quad (9.99)$$

We still require the conditions (9.95) and (9.96). On the basis of the foregoing discussion we expect the eikonal approximation to become progressively better since it includes the important term  $C(\Delta)/k^2$  which is proportional to  $U_0^3$ . This is indeed the case, as shown in Table 9.6 for a “double Yukawa” potential (9.89) with  $U_0 = 3$  and  $k = 5$ .

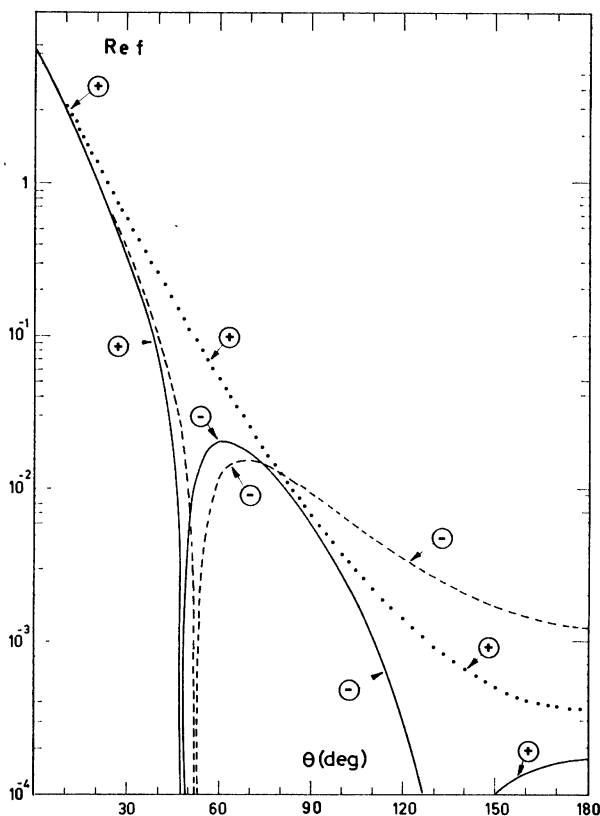


Fig. 9.6. The real part of the scattering amplitude for a polarization potential of the form  $U(r) = -U_0/(r^2 + d^2)^2$ , with  $U_0 = 10$ ,  $d = 1$  (unit of length) and  $k = 5$ . The solid curve shows the exact result, the dashed curve gives the eikonal result, and the dotted curve is the first Born approximation (taken from ref. [22]).

As another illustration of an “intermediate coupling” situation, where the value of  $|U_0|$  is still bigger, we show in Figs. 9.4 and 9.5 the real and imaginary parts of the exact, first Born, second Born and eikonal amplitudes for the interaction (9.89) with  $U_0 = 20$  and  $k = 5$ . We see that the eikonal result follows very closely the exact amplitude even at large angles, while the first and second Born approximations are consistently poorer.

Before leaving our discussion of intermediate coupling, we emphasize that the asymptotic relations (9.84) and (9.93) are valid for *all* momentum

transfers in the case of Yukawa-type potentials but *not* for all interactions. To illustrate this point, we compare in Figs. 9.6 and 9.7 the eikonal and exact results for a “polarization” potential of the form  $U(r) = -U_0/(r^2 + d^2)^2$ , with  $U_0 = 10$ ,  $d = 1$  (unit of length) and  $k = 5$ . Also shown for comparison in Fig. 9.6 are the first Born approximation values. We note that at small angles the agreement between the exact and eikonal results is excellent, but at larger angles this agreement does not persist.

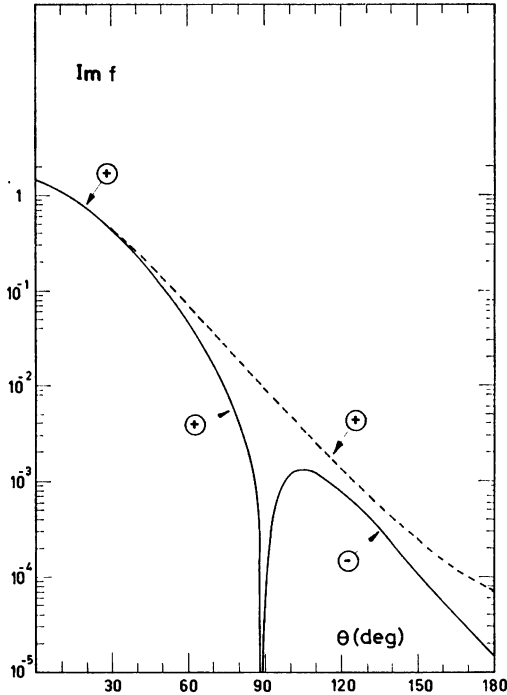


Fig. 9.7. The imaginary part of the scattering amplitude for a polarization potential of the form  $U(r) = -U_0/(r^2 + d^2)^2$ , with  $U_0 = 10$ ,  $d = 1$  and  $k = 5$ . The solid curve shows the exact result, the dashed curve gives the eikonal result (taken from ref. [22]).

It is also interesting to study what happens when we still increase the strength  $|U_0|$  of the potential so that  $|U_0|a/2k = |V_0|a/\hbar v \gg 1$ , with  $|U_0|/k^2 = |V_0|/E > 1$ . This is a *strong coupling* situation, for which the Born series is useless. Nevertheless, the eikonal approximation remains very accurate at small angles, provided that  $ka \gg 1$ . This is illustrated in Fig. 9.8, where we show the exact and the eikonal differential cross sections for a Yukawa potential of the form (9.77), with  $U_0 = 250$ ,  $a = \alpha^{-1} = 1$  and  $k = 5$ . This result is rather unexpected in view of the fact that the condition  $|V_0| \ll E$  has been required in order to obtain the eikonal wave function (9.29) [see Section 9.1.1]. However, we shall see in Section 9.2.4 that when  $ka \gg 1$  and

for *small angle* scattering, the eikonal scattering amplitude is equivalent to the amplitude obtained by using the WKB phase shift in the partial wave series, together with the approximate formula (9.41). The accuracy of the eikonal results for small angle, large wave number scattering by strong potentials then follows from the fact that the WKB method is precisely *exact* in the strong coupling limit (see Section 9.2).

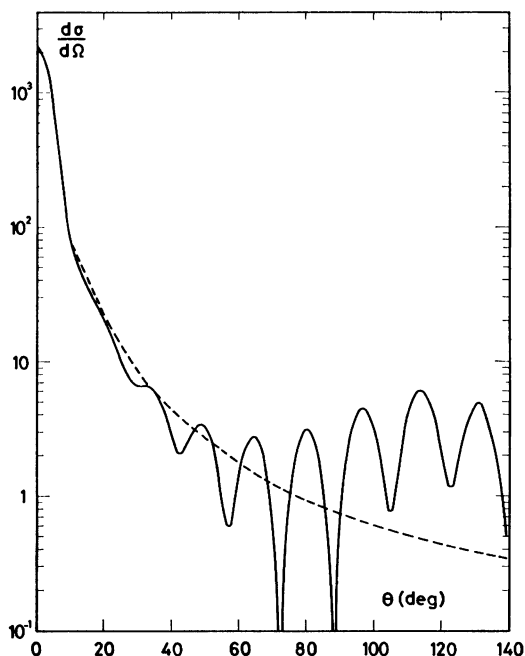


Fig. 9.8. The differential cross section for a Yukawa potential of the form (9.77), with  $U_0 = 250$ ,  $a = a^{-1} = 1$  (unit of length) and  $k = 5$ . The solid curve shows the exact result, the dashed curve gives the eikonal result.

## 9.2. The WKB Method

The Wentzel–Kramers–Brillouin [38–40] or WKB approximation was introduced in quantum mechanics in 1926, although the corresponding mathematical apparatus had been developed earlier by several authors [see e.g. 41]. As an introduction to the method, we shall first examine the classical limit of the Schrödinger equation. We then discuss the WKB approximation as applied to one-dimensional problems, in particular to the radial equation for the scattering by a central potential. We derive in this way the WKB radial wave functions and the corresponding phase shifts. The WKB scattering amplitude is then obtained by an approximate summation of the partial wave series.

### 9.2.1. The classical limit of the Schrödinger equation

Let us return to the time-dependent Schrödinger equation (3.21), namely

$$\left[ -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) \quad (9.100)$$

and look for a solution of the form

$$\Psi(\mathbf{r}, t) = A \exp \left[ \frac{i}{\hbar} W(\mathbf{r}, t) \right]. \quad (9.101)$$

The function  $W$  must then satisfy the equation

$$\frac{\partial W}{\partial t} + \frac{1}{2m} (\nabla_{\mathbf{r}} W)^2 + V - \frac{i\hbar}{2m} \nabla_{\mathbf{r}}^2 W = 0 \quad (9.102)$$

which in the classical limit ( $\hbar \rightarrow 0$ ) reduces to the Hamilton–Jacobi equation for the principal function  $W$ , namely

$$\partial W / \partial t + H(\mathbf{r}, \mathbf{p}) = 0. \quad (9.103)$$

Let us recall briefly the interpretation of eq. (9.103) within the framework of classical mechanics. For the one-body problem that we are considering, the function  $W$  depends on six integration constants. Since  $V$  is time-independent, these six parameters are the initial values (at  $t = t_0$ ) of the canonical coordinates  $\mathbf{r}$  and  $\mathbf{p}$ . A particular solution  $W$  of the Hamilton–Jacobi equation then describes completely a single classical trajectory. That is, the coordinates  $\mathbf{r}(t)$  may be inferred [42] from the knowledge of  $W$  and the momentum of the particle is given by

$$\mathbf{p}(t) = \nabla_{\mathbf{r}} W(\mathbf{r}, t). \quad (9.104)$$

From eq. (9.104) we see that in the classical limit the possible trajectories are orthogonal to the surfaces of constant phase  $W$ . As Hamilton observed in 1834, we may therefore interpret classical mechanics as the “geometrical optics” limit of a wave motion, the classical orbits or “rays” being orthogonal to the wave fronts  $W = \text{constant}$ . This idea was the starting point of the investigations of de Broglie [43] and Schrödinger [44], which led to the formulation of wave mechanics.

Let us now consider a stationary (energy) eigenfunction  $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp(-iEt/\hbar)$ . In this case we have

$$W(\mathbf{r}, t) = S(\mathbf{r}) - Et \quad (9.105)$$

and thus

$$\psi(\mathbf{r}) = A \exp \left[ \frac{i}{\hbar} S(\mathbf{r}) \right]. \quad (9.106)$$

Furthermore, eq. (9.102) now becomes

$$\frac{1}{2m} (\nabla_{\mathbf{r}} S)^2 - [E - V(\mathbf{r})] - \frac{i\hbar}{2m} \nabla_{\mathbf{r}}^2 S = 0. \quad (9.107)$$

In the classical limit ( $\hbar \rightarrow 0$ ) this equation reduces to

$$\frac{1}{2m}(\nabla_r S)^2 = E - V(r) \quad (9.108)$$

which is the equation determining Hamilton's characteristic function  $S$  in classical mechanics. We note that if we introduce the reduced de Broglie wavelength in the presence of the potential  $V(r)$ , namely

$$\lambda(r) = \hbar / \sqrt{2m[E - V(r)]} \quad (9.109)$$

we may also write eq. (9.108) as

$$(\nabla_r \hat{S})^2 = [\lambda(r)]^{-2} \quad (9.110)$$

where we have defined  $\hat{S}(r) = S(r)/\hbar$ . This equation is often called the *eikonal equation* [45–46] since it determines the phase (or eikonal) of the function (9.106). It is precisely the equation of wave fronts of geometrical optics. We note that when  $V = 0$  (i.e. for a free particle) a particular solution of eq. (9.110) is given by

$$\hat{S} = \mathbf{k} \cdot \mathbf{r} + \text{constant} \quad (9.111)$$

where  $\mathbf{k}$  is a given vector, of length  $k = \lambda^{-1}$ . The wave fronts are then planes perpendicular to  $\mathbf{k}$ , the rays being straight lines parallel to  $\mathbf{k}$ .

Let us now return to eq. (9.107) but without going to the limit  $\hbar \rightarrow 0$ . If

$$|\hbar(\nabla_r^2 S)| \ll |(\nabla_r S)^2| \quad (9.112)$$

we still expect eq. (9.108) to yield a useful approximation for the eikonal  $S$ . We shall call  $S_0$  this approximate expression of  $S$ . To analyze this point in more detail, let us consider a *one-dimensional example*. In this case eq. (9.108) may be integrated directly and yields

$$S_0(x) = \pm \int^x \sqrt{2m[E - V(x')]} dx' \quad (9.113)$$

so that, with the help of eqs. (9.106) and (9.109) we have

$$\psi(x) = A \exp\left(\pm i \int^x \kappa(x') dx'\right) \quad (9.114)$$

where

$$\kappa(x) = \lambda^{-1}(x) = \frac{1}{\hbar} \sqrt{2m[E - V(x)]} \quad (9.115)$$

is the “effective wave number”. Moreover, the condition (9.112) may now be written as

$$\left| \frac{d\lambda(x)}{dx} \right| / [\lambda(x)]^2 \ll |\lambda(x)|^{-2}. \quad (9.116)$$

Hence the *semi-classical wave function* (9.114) will be useful if

$$|d\lambda(x)/dx| \ll 1 \quad (9.117)$$



and provided that

$$\lambda(x) \neq \infty. \quad (9.118)$$

The condition (9.117) implies that the potential energy  $V(x)$  must change slowly over a distance comparable to the wavelength. The other condition (9.118) states that we must stay away from those points  $x_0$  for which  $V(x_0) = E$ . These are the classical *turning points*: the velocity of a classical particle vanishes and changes sign at  $x = x_0$ , so that in classical mechanics the particles never go beyond a turning point.

Let us consider again the semi-classical wave function (9.114). If we assume that  $E \gg |V(x)|$ , we may expand the effective wave number as

$$\kappa(x) = k \left[ 1 - \frac{1}{2} \frac{V(x)}{E} + \cdots \right] = k - \frac{U(x)}{2k} + \cdots \quad (9.119)$$

where  $k = (2mE)^{1/2}/\hbar$  and  $U(x) = 2mV(x)/\hbar^2$ . The semi-classical wave function (9.114) then becomes

$$\psi(x) = A \exp \left[ \pm i \left( kx - \frac{1}{2k} \int^x U(x') dx' \right) \right] \quad (9.120)$$

which is the one-dimensional analogue of the *eikonal* wave function (9.29).

### 9.2.2. The WKB Method in one dimension

We have thus far considered the reduction of eq. (9.107) to the classical equation (9.108). We may generalize this procedure by expanding the function  $S$  as a power series in  $\hbar$ ,

$$S = S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots \quad (9.121)$$

The WKB method obtains the first two terms of this expansion. We shall consider here the particular case of *one-dimensional problems*, for which the WKB approach can be easily applied. Thus, writing eq. (9.107) as

$$i\hbar S'' - S'^2 + 2m(E - V) = 0 \quad (9.122)$$

we find by substituting the expansion (9.121) into eq. (9.122) that

$$\begin{aligned} -S_0'^2 + 2m(E - V) &= 0, \\ iS_0'' - 2S_0'S_1' &= 0, \text{ etc.} \end{aligned} \quad (9.123)$$

The first of these equations gives the result (9.113) for  $S_0(x)$ , while the second equation yields for  $E > V$

$$S_1(x) = \frac{1}{2}i \log \kappa(x). \quad (9.124)$$

Thus, for  $E > V$ , we find that in the WKB approximation the wave function (9.106) has the form

$$\psi(x) = \frac{1}{\sqrt{\kappa(x)}} \left\{ A \exp \left[ i \int^x \kappa(x') dx' \right] + B \exp \left[ -i \int^x \kappa(x') dx' \right] \right\}. \quad (9.125)$$

Similarly, for  $E < V$  (i.e. in the classically forbidden region), one obtains

$$\psi(x) = \frac{1}{\sqrt{|\kappa(x)|}} \left\{ C \exp \left[ - \int^x |\kappa(x')| dx' \right] + D \exp \left[ \int^x |\kappa(x')| dx' \right] \right\}. \quad (9.126)$$

It is important to note that the wave functions (9.125) and (9.126) are “asymptotically” valid, since they may only be used several wavelengths away from the nearest turning point. A key problem of the WKB method is therefore to obtain *connection formulae* which allow one to join the two types of solutions (9.125) and (9.126) across a turning point. This interpolation is based on the fact that the original one-dimensional Schrödinger equation

$$d^2\psi/dx^2 + [k^2 - U(x)]\psi(x) = 0 \quad (9.127)$$

can be modified slightly so that an “exact” solution at and near a turning point may be written down [47]. This “exact” solution may then be joined smoothly on both sides of the turning point to the “asymptotic” wave functions obtained above. A detailed study of the connection formulae may be found in the references [48–52] listed at the end of this chapter.

### 9.2.3. The radial equation and the WKB phase shifts

Since the WKB approximation is simple in one-dimensional situations, it is natural to apply it to the solution of the radial equation (4.17), namely

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - U(r)]u_l(r) = 0. \quad (9.128)$$

We assume that the central potential  $U(r)$  decreases faster than  $r^{-1}$  as  $r \rightarrow \infty$  and is less singular than  $r^{-2}$  at  $r = 0$ .

We first make the change of variable

$$r = k^{-1} e^x \quad (9.129)$$

so that, as  $0 \leq r \leq \infty$ , we have  $-\infty \leq x \leq +\infty$ . We also define a new unknown function  $w(x)$  such that

$$u_l(r) = e^{x/2} w(x). \quad (9.130)$$

The radial equation (9.128) then becomes

$$d^2w/dx^2 + Q^2(x)w = 0 \quad (9.131)$$

where

$$Q^2(x) = e^{2x}(1 - U/k^2) - (l + \frac{1}{2})^2. \quad (9.132)$$

Now  $Q^2 > 0$  for  $x$  large and positive, while  $Q^2 < 0$  when  $|x|$  is large but  $x$  is negative. Let us assume that  $Q^2(x) = 0$  at one point  $x = x_0$ , which we also call a *turning point* [53]. Hence  $Q^2 > 0$  for  $x > x_0$  and  $Q^2 < 0$  for  $x < x_0$ .

To solve eq. (9.131), which is formally equivalent to the one-dimensional Schrödinger equation (9.127), we try the ansatz

$$w(x) = \frac{1}{\sqrt{q(x)}} \exp \left[ \pm i \int_{x_0}^x q(x') dx' \right] \quad (9.133)$$

where  $q(x)$  is an unknown function. Substituting into eq. (9.131) we find that

$$q^2(x) + R(x) = Q^2(x) \quad (9.134)$$

where

$$R(x) = q''/2q - \frac{3}{4}(q')^2/q^2 \quad (9.135)$$

and we have written  $q' \equiv dq/dx$ ,  $q'' \equiv d^2q/dx^2$ . The WKB approximation consists in neglecting the term  $R(x)$  in eq. (9.134). This is allowed provided that

$$|R(x)| \ll |Q^2(x)| \quad (9.136)$$

a condition which is satisfied when the potential changes slowly over a de Broglie wavelength of the incident particle. We also note that for fixed values of  $k$  and  $l$  the quantity  $|Q^2|$  increases with the strength of the potential, while the correction term  $|R|$  (as obtained by using the WKB ansatz  $q^2 = Q^2$ ) does not. Hence the WKB approximation  $q^2 = Q^2$  becomes exact in the *strong coupling* limit.

Adopting the WKB approximation, we see that for  $x > x_0$  the general solution of eq. (9.131) is given by [compare with eq. (9.125)]

$$w(x) = \frac{1}{\sqrt{Q}} \left\{ A \exp \left[ i \int_{x_0}^x Q(x') dx' \right] + B \exp \left[ -i \int_{x_0}^x Q(x') dx' \right] \right\}, \quad Q > 0, \quad x > x_0 \quad (9.137)$$

where  $A$  and  $B$  are constants. For  $x < x_0$  we have [compare with eq. (9.126)]

$$w(x) = \frac{1}{\sqrt{|Q|}} \left\{ C \exp \left[ - \int_{x_0}^x |Q(x')| dx' \right] + D \exp \left[ \int_{x_0}^x |Q(x')| dx' \right] \right\}, \quad Q < 0, \quad x < x_0 \quad (9.138)$$

where  $C$  and  $D$  are also two constants. Since  $u_l(0) = 0$  we must have  $w(x) = 0$  at  $x = -\infty$ . We therefore have to choose  $C = 0$ , so that

$$w(x) = \frac{1}{\sqrt{|Q|}} D \exp \left[ - \int_x^{x_0} |Q(x')| dx' \right], \quad Q < 0, \quad x < x_0. \quad (9.139)$$

At the turning point  $x = x_0$ , where the inequality (9.136) is no more valid, both expressions (9.137) and (9.139) of the function  $w(x)$  are inadequate. It is thus necessary to solve the original equation (9.131) – or a slightly modified version of it – around the point  $x = x_0$ . We shall follow here the treatment of Goldberger and Watson [54]. Let us assume that in the neighbourhood of  $x = x_0$  the function  $Q^2(x)$  may be written as

$$Q^2(x) = \alpha(x - x_0) \quad (9.140)$$

where  $\alpha$  is a non-vanishing constant. This is called the *linear turning point* approximation. Then, in the vicinity of  $x = x_0$ , eq. (9.131) becomes

$$d^2w/dy^2 + \alpha y w = 0 \quad (9.141)$$

where we have set  $y = x - x_0$ . This equation may be integrated explicitly and leads to the connection formulae [54]

$$A = -i \exp(\frac{1}{4}i\pi)D, \quad B = i \exp(-\frac{1}{4}i\pi)D. \quad (9.142)$$

Hence, for  $x > x_0$

$$w(x) = \frac{2D}{\sqrt{Q(x)}} \sin\left[\frac{1}{4}\pi + \int_{x_0}^x Q(x') dx'\right]. \quad (9.143)$$

We now return to our original variable  $r$ . Using eq. (9.129), we find that

$$Q^2(x) = r^2 F(r) \quad (9.144)$$

where we have set

$$F(r) = k^2 - U(r) - (l + \frac{1}{2})^2/r^2 \quad (9.145)$$

and the turning point at  $r_0 = k^{-1} \exp(x_0)$  is such that  $F(r_0) = 0$ . Then, since  $u_l(r) = [\exp(x/2)]w(x)$  and  $\exp(x/2) = (kr)^{1/2}$ , we have for  $r > r_0$

$$u_l(r) = (kr)^{1/2}w = 2[k^2/F(r)]^{1/4}D \sin\left[\frac{1}{4}\pi + \int_{r_0}^r F^{1/2}(r') dr'\right]. \quad (9.146)$$

To find the phase shifts  $\delta_l$ , we take the limit  $r \rightarrow \infty$ . As  $F(r) \rightarrow k^2$  for  $r \rightarrow \infty$ , we have

$$u_l(r) \xrightarrow{r \rightarrow \infty} 2D \sin\left\{\frac{1}{4}\pi + \int_{r_0}^{\infty} [F^{1/2}(r') - k] dr' + k(r - r_0)\right\}. \quad (9.147)$$

The constant  $D$  is seen to fix the "normalization" of the wave function. On the other hand, by comparing eq. (9.147) with the asymptotic form of the radial function, namely

$$u_l(r) \xrightarrow{r \rightarrow \infty} A_l \sin(kr - \frac{1}{2}l\pi + \delta_l), \quad (9.148)$$

one obtains the WKB phase shifts

$$\delta_l^{\text{WKB}} = (l + \frac{1}{2})\frac{1}{2}\pi - kr_0 + \int_{r_0}^{\infty} [F^{1/2}(r) - k] dr. \quad (9.149)$$

After integrating by parts and remembering that  $F(r_0) = 0$ , we also have

$$\delta_l^{\text{WKB}} = (l + \frac{1}{2})\frac{1}{2}\pi - \int_{r_0}^{\infty} r \frac{d}{dr} [F^{1/2}(r)] dr. \quad (9.150)$$

Let us analyze a few properties of the WKB phase shifts. First of all, we verify from eq. (9.150) that  $\delta_l^{\text{WKB}} = 0$  when  $U(r) = 0$ . Indeed in that case we have  $F(r) = k^2 - (l + \frac{1}{2})^2/r^2$  and the corresponding turning point, which we call  $r_1$ , is given by  $r_1 = (l + \frac{1}{2})/k$ . The integral appearing on the right-hand side of eq. (9.150) then reduces to

$$\int_{r_1}^{\infty} r \frac{d}{dr} \left[ k^2 - \frac{(l + \frac{1}{2})^2}{r^2} \right]^{1/2} dr = (l + \frac{1}{2}) \int_0^{\infty} \text{sech } t \, dt = (l + \frac{1}{2})\frac{1}{2}\pi \quad (9.151)$$

where we have made the change of variables  $r = r_1 \cosh t$  and used the fact that  $\int \operatorname{sech} t \, dt = 2 \tan^{-1}[\exp(t)]$ . The result (9.151) also allows us to recast the WKB phase shift (9.150) in the form

$$\delta_l^{\text{WKB}} = \int_{r_1}^{\infty} r \frac{d}{dr} \left[ k^2 - \frac{(l + \frac{1}{2})^2}{r^2} \right]^{1/2} dr - \int_{r_0}^{\infty} r \frac{d}{dr} \left[ k^2 - \frac{(l + \frac{1}{2})^2}{r^2} - U(r) \right]^{1/2} dr. \quad (9.152)$$

It is worth recalling at this point that in applying the WKB method we have already assumed that the *short wavelength* condition  $ka \gg 1$  is satisfied (for a potential having a “range”  $a$ ). Moreover, as we shall see below, quasi-classical scattering is dominated by *large values of  $l$* . The magnitude  $L$  of the angular momentum is then given by  $\hbar\sqrt{l(l+1)} \simeq \hbar(l + \frac{1}{2})$ . In what follows we shall write

$$L = \hbar(l + \frac{1}{2}). \quad (9.153)$$

Hence the expression (9.149) for  $\delta_l^{\text{WKB}}$  becomes

$$\delta_l^{\text{WKB}} = \frac{L\pi}{2\hbar} - kr_0 + \hbar^{-1} \int_{r_0}^{\infty} \left\{ \left[ 2m[E - V(r)] - \frac{L^2}{r^2} \right]^{1/2} - \hbar k \right\} dr. \quad (9.154)$$

If we treat  $l$  as a continuous variable and differentiate eq. (9.154) with respect to it, we obtain with the help of eq. (9.153)

$$\partial \delta_l^{\text{WKB}} / \partial l = \hbar \partial \delta_l^{\text{WKB}} / \partial L = \frac{1}{2} \Theta \quad (9.155)$$

where

$$\begin{aligned} \Theta &= \pi + 2 \int_{r_0}^{\infty} \frac{\partial}{\partial L} \left\{ 2m[E - V(r)] - \frac{L^2}{r^2} \right\}^{1/2} dr \\ &= \pi - 2 \int_{r_0}^{\infty} r^{-2} \{ 2m[E - V(r)] L^{-2} - r^{-2} \}^{-1/2} dr \end{aligned} \quad (9.156)$$

is the *classical angle of deflection* [55, 56].

Another important property of the WKB phase shift follows from the fact [already pointed out after eq. (9.136)] that the WKB method becomes exact in the strong coupling limit. Thus the WKB phase shift  $\delta_l^{\text{WKB}}$  is the limiting value of  $\delta_l$  when the strength  $|U_0|$  of the potential becomes large.

Let us now return to the expression (9.152) of the WKB phase shift. For *large  $l$*  (and fixed  $k$ ), the value of  $r_0$  also becomes large and the potential  $U(r)$  remains small over the integration range  $(r_0, \infty)$ . We may therefore expand the quantity  $F^{1/2}(r)$  as

$$\begin{aligned} F^{1/2}(r) &= [k^2 - (l + \frac{1}{2})^2/r^2 - U(r)]^{1/2} \\ &= \left[ k^2 - \frac{(l + \frac{1}{2})^2}{r^2} \right]^{1/2} \left\{ 1 - \frac{U(r)}{2[k^2 - (l + \frac{1}{2})^2/r^2]} + \cdots \right\}. \end{aligned} \quad (9.157)$$

Moreover, we also have in this case

$$r_0 \simeq r_1 = (l + \frac{1}{2})/k. \quad (9.158)$$

We then obtain from eq. (9.152), after integrating by parts and using the relations (9.157) and (9.158),

$$\delta_l^{\text{WKB}}(k) \simeq -\frac{1}{2k} \int_{(l+\frac{1}{2})/k}^{\infty} \frac{rU(r)}{[r^2 - (l + \frac{1}{2})^2/k^2]^{1/2}} dr. \quad (9.159)$$

We note that this integral converges if  $U(r)$  tends to zero faster than  $r^{-1}$  as  $r \rightarrow \infty$ .

We now remark that according to eq. (9.43) the *impact parameter*  $b$  is given by  $b \simeq (l + \frac{1}{2})/k$ . Hence we may write eq. (9.159) in the form

$$\delta_l^{\text{WKB}}(k) \simeq -\frac{1}{2k} \int_b^{\infty} \frac{rU(r)}{\sqrt{r^2 - b^2}} dr, \quad l + \frac{1}{2} = kb. \quad (9.160)$$

Changing the integration variable from  $r$  to  $z = \sqrt{r^2 - b^2}$  and using the fact that  $U(b, z) = U(b, -z)$  we finally obtain (for large  $l$  and  $ka \gg 1$ )

$$\delta_l^{\text{WKB}}(k) \simeq -\frac{1}{4k} \int_{-\infty}^{+\infty} U(b, z) dz, \quad l + \frac{1}{2} = kb \quad (9.161)$$

which is the *eikonal phase shift* (9.46).

TABLE 9.7

Comparison of the eikonal, WKB and exact phase shifts  $\delta_l$  (in radians), for attractive "polarization" potentials of the form  $U(r) = -U_0/(r^2 + d^2)^2$ , with  $d = 1$  (unit of length) and various values of  $l$ . The wave number is  $k = 5$ . The numbers in parentheses indicate powers of 10.

$l$	$U_0 = 1$			$U_0 = 250$		
	Eikonal	WKB	Exact	Eikonal	WKB	Exact
0	7.74 (−2)	7.69 (−2)	7.80 (−2)	1.93 (1)	1.14 (1)	1.14 (1)
1	6.90 (−2)	6.89 (−2)	6.90 (−2)	1.73 (1)	1.12 (1)	1.12 (1)
2	5.62 (−2)	5.63 (−2)	5.59 (−2)	1.40 (1)	1.09 (1)	1.09 (1)
3	4.32 (−2)	4.33 (−2)	4.29 (−2)	1.08 (1)	1.04 (1)	1.04 (1)
4	3.23 (−2)	3.24 (−2)	3.21 (−2)	8.06	9.78	9.78
5	2.39 (−2)	2.40 (−2)	2.38 (−2)	5.98	8.95	8.96
6	1.78 (−2)	1.79 (−2)	1.78 (−2)	4.45	7.94	7.94
7	1.34 (−2)	1.34 (−2)	1.34 (−2)	3.25	6.71	6.70
8	1.02 (−2)	1.03 (−2)	1.03 (−2)	2.56	5.25	5.23
9	7.93 (−3)	7.95 (−3)	7.95 (−3)	1.98	3.61	3.56
10	6.24 (−3)	6.26 (−3)	6.26 (−3)	1.56	2.32	2.31
15	2.27 (−3)	2.28 (−3)	2.28 (−3)	5.68 (−1)	6.17 (−1)	6.19 (−1)
20	1.04 (−3)	1.05 (−3)	1.05 (−3)	2.61 (−1)	2.69 (−1)	2.69 (−1)
25	5.60 (−4)	5.60 (−4)	5.60 (−4)	1.40 (−1)	1.42 (−1)	1.42 (−1)

As an example, we show in Table 9.7 the values of the phase shifts  $\delta_l$  obtained from the eikonal approximation [see eq. (9.161)], those corresponding to the WKB formula (9.149), and the exact values, obtained from a

numerical integration of the radial equation (4.17). This comparison is made for "polarization" potentials of the form  $U(r) = -U_0/(r^2 + d^2)^2$ , with  $d = 1$  (unit of length),  $k = 5$  and two coupling strengths  $U_0 = 1$  and  $U_0 = 250$ . We note that in the *weak coupling* situation ( $U_0 = 1$ ) both the eikonal and the WKB phase shifts agree very well with the exact results for all values of  $l$ . For the *strong coupling* case ( $U_0 = 250$ ) the WKB phase shifts are accurate for all values of  $l$ , while the eikonal phase shifts are only reliable for large  $l$ -values.

#### 9.2.4. The scattering amplitude

Having obtained the WKB phase shifts, one may insert them in the partial wave series (4.63), namely

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \{\exp(2i\delta_l) - 1\} P_l(\cos \theta). \quad (9.162)$$

In what follows we shall sum this series approximately by using the fact that we are in the semi-classical regime. Since  $ka \gg 1$ , large  $l$  values (of the order of  $ka$ ) dominate the scattering. For *small scattering angles* such that  $l\theta = \mathcal{O}(1)$  we may use eq. (9.41) and turn the sum on  $l$  into an integral on the impact parameter  $b$  [see eq. (9.44)]. Because of the result (9.161) we then obtain the *eikonal scattering amplitude* (9.40). We emphasize that this procedure is justified for scattering angles  $\theta \lesssim l^{-1} \simeq (ka)^{-1}$  which correspond to diffraction scattering.

Let us now consider the angular region  $\theta > (ka)^{-1}$ . We first observe that the closure relation for the Legendre polynomials yields [see eq. (B.6) of Appendix B]

$$\frac{1}{2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) P_l(1) = \delta(\cos \theta - 1) \quad (9.163)$$

so that the term in the partial wave series (9.162) which does not contain the phase shift only contributes in the forward direction. Since we are excluding the angular range  $0 \leq \theta \leq (ka)^{-1}$ , we may therefore omit this term and write

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \exp(2i\delta_l) P_l(\cos \theta), \quad \theta \neq 0. \quad (9.164)$$

We shall study this expression in the *quasi-classical* limit. In this case, the phases  $\delta_l$  are large and the terms with large  $l$ -values dominate the sum [51]. We may then use the asymptotic (large  $l$ ) form of  $P_l(\cos \theta)$ , namely [see e.g. 57]

$$P_l(\cos \theta) \approx \left[ \frac{2}{\pi l \sin \theta} \right]^{1/2} \sin \left[ \left( l + \frac{1}{2} \right) \theta + \frac{1}{4} \pi \right]. \quad (9.165)$$

This approximation is valid for  $l > (\sin \theta)^{-1}$ . Hence, since large  $l$  values (of the order of  $ka$ ) are the dominant ones, this approach is suitable for scattering angles  $\theta$  larger than  $(ka)^{-1}$ , i.e. those which we are presently considering. We thus have from eqs. (9.164) and (9.165)

$$f(\theta) = -\frac{1}{k} \int_0^\infty \left[ \frac{l}{2\pi \sin \theta} \right]^{1/2} [\exp(i\phi_+) - \exp(i\phi_-)] dl \quad (9.166)$$

where we have treated  $l$  as a continuous variable and set

$$\phi_\pm = 2\delta_l \pm (l + \frac{1}{2})\theta \pm \frac{1}{4}\pi. \quad (9.167)$$

The exponential terms appearing in eq. (9.166) are rapidly oscillating, since the phases  $\phi_\pm$  are large. Thus effectively the scattering amplitude (9.166) is determined by the range of  $l$ -values for which the quantities  $\phi_\pm$  have an extremum. These values of  $l$  therefore lie in the neighbourhood of the roots  $l = l_i$  of the equation

$$\partial\phi_\pm/\partial l = 0 \quad (9.168)$$

or

$$2\partial\delta_l/\partial l \pm \theta = 0. \quad (9.169)$$

Let us assume that there is *one* root of eq. (9.168) at a large value  $l = l_0$ . We then have in the neighbourhood of this value

$$\phi_\pm(l) = \phi_\pm(l_0) + \beta_\pm(l_0)(l - l_0)^2 \quad (9.170)$$

with

$$\beta_\pm(l_0) = \frac{1}{2}[\partial^2\phi_\pm/\partial l^2]_{l=l_0} \quad (9.171)$$

and the scattering amplitude (9.166) becomes

$$f(\theta) = -\frac{1}{k} \left\{ \frac{l_0}{2\pi \sin \theta} \right\}^{1/2} \exp\{i\phi_\pm(l_0)\} \int_{l_0-\Delta l}^{l_0+\Delta l} \exp\{i\beta_\pm(l_0)(l - l_0)^2\} dl \quad (9.172)$$

where we have indicated explicitly that the main contribution to the integral arises from the interval  $(l_0 - \Delta l, l_0 + \Delta l)$  centered about the value  $l = l_0$ . We may now change variables from  $l$  to  $\xi = l - l_0$  and extend without appreciable error the integral from  $-\infty$  to  $+\infty$ . This yields

$$f(\theta) = -\frac{1}{k} \left\{ \frac{l_0}{2\pi \sin \theta} \right\}^{1/2} \left\{ \frac{\pi}{i\beta_\pm(l_0)} \right\}^{1/2} \exp\{i\phi_\pm(l_0)\}. \quad (9.173)$$

Before we discuss in more detail this expression, let us come back to the relation (9.169). From the results (9.155) and (9.156) we see that if we use the WKB phase shifts  $\delta_l^{\text{WKB}}$  we obtain from this relation the *classical* result

$$\int_{r_0}^\infty \frac{\partial}{\partial L} \left[ 2m[E - V(r)] - \frac{L^2}{r^2} \right]^{1/2} dr + \frac{1}{2}\pi \pm \frac{1}{2}\theta = 0 \quad (9.174)$$

or

$$\theta = \pm \Theta(l_0) \quad (9.175)$$



where the choice of sign is determined by the fact that the scattering angle  $\theta$  is always positive. The classical deflection angle  $\Theta$  is positive for a repulsive interaction and negative for an attractive one. We shall call  $L_0 = (l_0 + \frac{1}{2})\hbar$  the root of eq. (9.174). Moreover, we also have from eqs. (9.155), (9.167) and (9.171)

$$\beta_{\pm}(l_0) = \frac{1}{2}[\partial\Theta/\partial l]_{l=l_0} = (\hbar/2)[\partial\Theta/\partial L]_{L=L_0}. \quad (9.176)$$

Let us now return to the scattering amplitude (9.173). In terms of  $L_0$ , we may write the corresponding cross section as

$$d\sigma/d\Omega = |f(\theta)|^2 = (L_0/p^2 \sin \theta) |dL_0/d\theta| \quad (9.177a)$$

or

$$d\sigma/d\Omega = (b_0/\sin \theta) |db_0/d\theta| \quad (9.177b)$$

where  $p$  is the magnitude of the particle momentum and we have used the fact that  $L_0 = b_0 p$  with  $kb_0 \simeq l_0$ . The differential cross section given by eqs. (9.177) [compare with eq. (4.79)] is simply the *classical* cross section  $d\sigma_{cl}/d\Omega$ . We note from the above derivation that the conditions for classical scattering through a given angle  $\theta$  are that the value  $l_0$  should be large and that  $\delta_l$  should also be large for this value. We also assumed that there was only *one* stationary point at  $l = l_0$ , which upon using eq. (9.175) means that  $\Theta(l)$  should be a monotonic function of  $l$  such that  $0 \leq \Theta(l) \leq \pi$ . If this is not the case one may obtain angular distributions which differ considerably from the classical one, even though the semi-classical conditions are satisfied. These more complicated situations, leading to “interference scattering”, “rainbow scattering”, “glory scattering”, etc. have been analyzed by Ford and Wheeler [58]. An outline of this subject may also be found in the references [59–61].

In the derivation leading to the classical result (9.177) we assumed that the scattering angle  $\theta$  should be such that  $\theta > (ka)^{-1}$ . It is easy to see why this condition holds. Indeed, a classical trajectory is only well defined if the uncertainty  $\Delta\theta$  in the scattering angle  $\theta$  is small compared to  $\theta$  itself. Now the uncertainty  $\Delta p$  in the transverse momentum of the scattered particle, as given by the Heisenberg uncertainty principle, is of the order of

$$\Delta p \sim \hbar/a. \quad (9.178)$$

The corresponding uncertainty  $\Delta\theta$  in the scattering angle is therefore given by

$$\Delta\theta \sim \Delta p/p \sim (ka)^{-1} \quad (9.179)$$

which implies that the scattering through sufficiently small angles  $\theta < (ka)^{-1}$  is never classical.

We may also express the above idea in a more quantitative way by obtaining first an estimate of  $\theta$  and then writing the condition  $\Delta\theta \ll \theta$  for classical scattering. Since in the short wavelength limit ( $ka \gg 1$ ) which we are considering the bulk of the scattering occurs near the forward direction we shall

assume that  $\theta$  is small [62]. Now the (small) deflection angle of a classical particle is roughly equal to

$$\theta \simeq \delta p/p \quad (9.180)$$

where  $\delta p$ , the momentum transfer in the transverse direction, is given in order of magnitude by the force  $V_0/a$  acting on the particle, multiplied by the "collision time"  $a/v$  (where  $v$  is the magnitude of the particle velocity). Hence

$$\theta \simeq |V_0|/pv = |V_0|/2E. \quad (9.181)$$

Using the relations (9.179) and (9.181) the condition  $\Delta\theta \ll \theta$  for classical scattering yields

$$|V_0|a/\hbar v = |U_0|a/2k \gg 1. \quad (9.182)$$

We note that the condition (9.182) for classical scattering corresponds to a *strong coupling* situation in which the coupling parameter  $|V_0|a/\hbar v$  is large [63]. This is in contrast with the condition of validity (8.65) of the first Born approximation which requires that  $|V_0|a/\hbar v \ll 1$ .

## References and notes

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- [36] Interaction potentials for which the relation (9.84) only holds at small angles include for example the gaussian potential  $U(r) = -U_0 \exp(-ar^2)$  and the "polarization" potential  $U(r) = -U_0/(r^2 + d^2)^2$  [where  $d$  is a fixed parameter having the dimensions of a length]. Details may be found in ref. [22] (Appendix B). See also ref. [23].
- [37] The relations (9.92) were first suggested by BYRON, JOACHAIN and MUND [21, 22] on the basis of an analysis of the first few terms (up to  $n = 4$ ) of the Born and eikonal series. MOORE [18] has shown that for a Yukawa potential (and by a direct extension for a superposition of Yukawa potentials) the first term in  $A_{Bn}(\Delta)$ , which is proportional to  $\log^{n-1} \Delta/\Delta^2$ , is equal to the first term in  $A_{En}(\Delta)$ . However, for Yukawa-type interactions the quantities  $A_{Bn}(\Delta)$  and  $A_{En}(\Delta)$  are linear combinations of terms of the form  $\log^m \Delta/\Delta^2$ , with  $0 \leq m \leq n-1$ , so that a general proof of eq. (9.92) is much more involved.
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## Variational Methods

In this chapter we shall study the application of variational methods to scattering problems. First of all, we recall that by writing the variational principle

$$\delta J = 0 \quad (10.1)$$

one expresses the fact that a certain functional  $J$ , characteristic of the system considered, is stationary for a “natural” system [1]. This property leads to the well-known Euler–Lagrange equations of the system.

The aim of (direct) variational methods is to search for solutions of the variational problem (10.1) among trial functions which depend on a finite number of variational parameters  $\alpha_1, \alpha_2, \dots, \alpha_n$ . The original *functional*  $J$  then becomes a *function*  $J(\alpha_1, \alpha_2, \dots, \alpha_n)$  of the variational parameters and the stationary property (10.1) yields the system of equations

$$\partial J / \partial \alpha_i = 0 \quad (i = 1, 2, \dots, n) \quad (10.2)$$

to determine the “best” parameters  $\alpha_1^0, \alpha_2^0, \dots, \alpha_n^0$ . Thus, by solving directly the variational problem in a restricted functional space, variational methods provide a powerful way of obtaining approximate solutions to the corresponding Euler–Lagrange equations, i.e. to a variety of differential and integral equations. By virtue of eq. (10.2), the value of the functional for the “best” parameters, namely

$$J_0 = J(\alpha_1^0, \alpha_2^0, \dots, \alpha_n^0) \quad (10.3)$$

is *correct to first order* when variations are imposed on the trial functions considered. This last property is of great importance in performing practical calculations, since the functional  $J$  is thus relatively insensitive to errors made in the trial functions.

Since the early developments of quantum theory, variational methods have proved to be very useful for solving bound state problems. It was only much later that the application of variational principles to quantum collision phenomena was proposed by Hulthén [2, 3], Tamm [4], Schwinger [5] and Kohn [6]. Numerous related methods have followed their work [7].

It is convenient to classify variational principles into *differential* or *integral* forms. The various differential forms are based directly on differential equations and require trial functions satisfying the boundary conditions of the problem. In the case of integral forms, the Euler–Lagrange equations are integral equations and therefore the boundary conditions, being taken into account through the Green’s functions, need not be incorporated in the trial functions.

In Section 10.1, we study the Hulthén–Kohn variational principle [2, 3, 6] which is currently the most widely used method based on the *differential* aspect of variational principles for collision processes. Section 10.2 is devoted to the Schwinger variational principles [5, 8–12] relying on the corresponding integral equations. Finally, in Section 10.3, we consider the important problem of *minimum* principles in scattering theory.

## 10.1. The Hulthén–Kohn variational principle

### 10.1.1. Variational principles for phase shifts

We consider the non-relativistic scattering of a spinless particle of mass  $m$  by a real potential  $V(r)$ . The exact radial function, which we denote here by  $\bar{u}_l(r)$ , satisfies the radial equation

$$L_l[\bar{u}_l] \equiv [d^2/dr^2 + k^2 - l(l+1)/r^2 - U(r)]\bar{u}_l(r) = 0 \quad (10.4)$$

where  $U(r) = 2mV(r)/\hbar^2$  is the reduced potential. In addition

$$\bar{u}_l(0) = 0 \quad (10.5)$$

and at large distances, we “normalize”  $\bar{u}_l(r)$  in such a way that

$$\bar{u}_l(r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi + \bar{\eta}_l) \quad (10.6)$$

where  $\bar{\eta}_l$  denotes the exact phase shift. The symbol  $\eta$  will be used throughout this chapter to denote phase shifts, in order to avoid any confusion with the variation symbol  $\delta$ . Barred quantities are exact.

Consider now the functional

$$I_l[u_l] = \int_0^\infty u_l(r) L_l[u_l(r)] dr. \quad (10.7)$$

We note that  $I_l = 0$  when  $u_l = \bar{u}_l$ . Let us adopt a trial function  $u_l(r)$  such that

$$u_l(r) = \bar{u}_l(r) + \delta u_l(r) \quad (10.8)$$

and satisfying the same boundary conditions as  $\bar{u}_l(r)$ . That is

$$u_l(0) = 0 \quad (10.9)$$

and

$$u_l(r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi + \eta_l) \quad (10.10)$$

where  $\eta_l$  is a trial phase shift. Hence

$$\delta u_l(0) = 0 \quad (10.11)$$

and

$$\delta u_l(r) \xrightarrow{r \rightarrow \infty} \cos(kr - \frac{1}{2}l\pi + \eta_l)\delta\eta_l. \quad (10.12)$$

We now calculate the variation  $\delta I_l$  of the functional  $I_l$ . We first have

$$\delta I_l = \int_0^\infty (\bar{u}_l(r) + \delta u_l(r))L_l[\bar{u}_l(r) + \delta u_l(r)] dr - \int_0^\infty \bar{u}_l(r)L_l[\bar{u}_l(r)] dr. \quad (10.13)$$

Using eq. (10.4) and the fact that  $L_l$  is a linear operator (i.e.  $L_l[\bar{u}_l + \delta u_l] = L_l[\bar{u}_l] + L_l[\delta u_l]$ ), we find that

$$\delta I_l = \int_0^\infty \bar{u}_l(r)L_l[\delta u_l(r)] dr + \int_0^\infty \delta u_l(r)L_l[\delta u_l(r)] dr. \quad (10.14)$$

Neglecting the second term on the right-hand side of eq. (10.14) since it is of second order in  $\delta u_l$ , and using Green's theorem [13], we have

$$\delta I_l = \left[ \bar{u}_l(r) \frac{d}{dr} \delta u_l(r) - \delta u_l(r) \frac{d}{dr} \bar{u}_l(r) \right]_0^\infty. \quad (10.15)$$

Hence, using eqs. (10.5)–(10.6) and (10.11)–(10.12), we obtain

$$\delta I_l = -k\delta\eta_l \quad (10.16)$$

so that the functional

$$J_l = I_l + k\eta_l \quad (10.17)$$

is stationary [ $\delta J_l = \delta(I_l + k\eta_l) = 0$ ]. Using this stationary property we may write

$$\bar{I}_l + k\bar{\eta}_l - I_l - k\eta_l + \dots = 0 \quad (10.18)$$

where second (and higher) order terms have been neglected. Since  $\bar{I}_l = 0$ , the variational phase shift which we shall denote by  $[\eta_l]$  is therefore given by

$$[\eta_l] = \eta_l + k^{-1}I_l. \quad (10.19)$$

In actual calculations, one starts from a trial function  $u_l(c_1, c_2, \dots, c_n; \eta_l; r)$  depending on  $(n + 1)$  parameters [namely  $c_1, c_2, \dots, c_n$  and the trial phase shift  $\eta_l$ ], and satisfying the boundary conditions (10.9)–(10.10). One then calculates  $J_l(c_1, c_2, \dots, c_n; \eta_l)$  and the  $(n + 1)$  parameters are determined by solving the system of  $(n + 1)$  equations

$$\begin{aligned} \frac{\partial}{\partial c_i} J_l &= 0 \quad (i = 1, 2, \dots, n) \\ \frac{\partial}{\partial \eta_l} J_l &= 0 \end{aligned} \quad (10.20)$$

or

$$\begin{aligned}\frac{\partial}{\partial c_i} I_l &= 0 \quad (i = 1, 2, \dots, n) \\ \frac{\partial}{\partial \eta_l} I_l &= -k.\end{aligned}\tag{10.21}$$

The trial phase shift  $\eta_l$  being determined in this way, the “variationally correct” phase shift  $[\eta_l]$  (second order accurate) is then obtained from eq. (10.19).

Slightly different variational principles can be written down with different “normalizations” for the functions  $\bar{u}_l(r)$  and  $u_l(r)$ . For example, with

$$\bar{u}_l(r) \xrightarrow{r \rightarrow \infty} \sin(kr - \tfrac{1}{2}l\pi) + \bar{\lambda}_l \cos(kr - \tfrac{1}{2}l\pi)\tag{10.22}$$

and

$$u_l(r) \xrightarrow{r \rightarrow \infty} \sin(kr - \tfrac{1}{2}l\pi) + \lambda_l \cos(kr - \tfrac{1}{2}l\pi)\tag{10.23}$$

where  $\bar{\lambda}_l = \tan \bar{\eta}_l$  and  $\lambda_l = \tan \eta_l$ , one gets

$$\delta(I_l + k\lambda_l) = 0.\tag{10.24}$$

In this case the equation

$$[\lambda_l] = \lambda_l + k^{-1}I_l\tag{10.25}$$

replaces eq. (10.19). The variational principle (10.24) is more convenient to use in practice than the corresponding variational principle (10.16) because the quantity  $\lambda_l$  appears as a *linear* parameter in the trial function. The Hulthén-Kohn procedure leading to eqs. (10.20)–(10.21) is unchanged, with now  $J_l = I_l + k\lambda_l$ . Hence one must solve the system of  $(n + 1)$  equations

$$\begin{aligned}\frac{\partial}{\partial c_i} I_l &= 0 \quad (i = 1, 2, \dots, n) \\ \frac{\partial}{\partial \lambda_l} I_l &= -k.\end{aligned}\tag{10.26}$$

As a particular case of eq. (10.25) we may easily derive a Hulthén-Kohn variational principle for the *scattering length*

$$\alpha = - \lim_{k \rightarrow 0} \tan \eta_0(k)/k.\tag{10.27}$$

Indeed, dividing eq. (10.25) by  $(-k)$  after setting  $l = 0$ , we find that

$$\left[ - \frac{\tan \eta_0(k)}{k} \right] = - \frac{\tan \eta_0(k)}{k} - \int_0^\infty \frac{u_0(k, r)}{k} L_0 \left[ \frac{u_0(k, r)}{k} \right] dr\tag{10.28}$$

where we have used eq. (10.7) and we have explicitly displayed the  $k$ -dependence of the function  $u_0$ . Let us now introduce the function

$$u^0(r) = \lim_{k \rightarrow 0} A(k)u_0(k, r)\tag{10.29}$$



where the superscript refers to the fact that  $k = 0$ , and  $A(k)$  is a “normalization” constant. We shall choose  $A(k) = -1/k$  so that from eqs. (10.23) and (10.29) we deduce that

$$u^0(r) \xrightarrow{r \rightarrow \infty} \alpha - r. \quad (10.30)$$

We now come back to eq. (10.28) in which we let  $k \rightarrow 0$ . We then find that

$$[\alpha] = \alpha - \int_0^\infty u^0(r) L_0[u^0(r)] dr \quad (10.31)$$

which is the desired variational principle for the scattering length.

Let us illustrate the variational principles (10.25) and (10.31) on a simple example. We consider a square well potential simulating low-energy neutron-proton scattering in the  ${}^3S_1$  state. That is,

$$U(r) = \begin{cases} -U_0, & r < a \\ 0, & r > a \end{cases} \quad (10.32)$$

with  $U_0 = 0.855 \text{ fm}^{-2}$  and  $a = 2.04 \text{ fm}$  [14], ( $1 \text{ fm} = 10^{-13} \text{ cm}$ ).

We first examine s-wave scattering at zero energy. The *exact* scattering length  $\bar{\alpha}$  is then given by eq. (4.157). This yields in our case

$$\bar{\alpha} = 5.3708 \text{ fm}. \quad (10.33)$$

To apply the Hulthén-Kohn variational principle (10.31) we choose a trial function of the type

$$u^0(r) = \begin{cases} \sum_{i=1}^N c_i r^i, & \text{for } r < a \\ \alpha - r, & \text{for } r > a \end{cases} \quad (10.34)$$

where  $c_i$  and  $\alpha$  are variational parameters. The conditions of continuity of the function  $u^0(r)$  and of its first derivative at  $r = a$  yield two constraints, so that the number of *free* parameters is  $(N - 1)$ . Table 10.1 gives the values of  $[\alpha]$  for several values of  $N$ . It is seen that a very accurate value of the scattering length is readily obtained with very simple trial functions.

TABLE 10.1

Variational calculation of the scattering length for the square well potential (10.32), using the Hulthén-Kohn variational principle (10.31). The trial function used is given by eq. (10.34). The exact scattering length  $\bar{\alpha}$  is given by  $\bar{\alpha} = 5.3708 \text{ fm}$ .

$N$	$[\alpha]$ in fm
1	-2.4161
2	5.5448
3	5.3810
4	5.3709
5	5.3708

Let us now consider s-wave scattering by the same square well (10.32), but for  $k = 0.25$ . We choose a trial function of the form

$$u_0(r) = \begin{cases} \sum_{i=1}^N c_i r^i & \text{for } r < a \\ \sin kr + \lambda_0 \cos kr & \text{for } r > a \quad (\lambda_0 = \tan \eta_0) \end{cases} \quad (10.35)$$

where  $c_i$  and  $\lambda_0$  are variational parameters. This function is “normalized” according to eq. (10.23). The variational principle (10.25) then yields for  $[\lambda_0]$  the values listed in Table 10.2 for several choices of  $N$ . The *exact* value  $\bar{\lambda}_0$ , obtained by using eq. (4.154) is given by  $\bar{\lambda}_0 = -1.9010$ . We note that, as in the preceding case, a variational value correct to five significant figures is obtained by using a simple trial function with only four free parameters.

TABLE 10.2

Variational calculation of the quantity  $\lambda_0 = \tan \eta_0$  for the square well potential (10.32), using the Hulthén-Kohn variational principle (10.25). The trial function used is that of eq. (10.35). The exact value is  $\bar{\lambda}_0 = -1.9010$

$N$	$[\lambda_0] = [\tan \eta_0]$
1	0.4768
2	-1.9982
3	-1.9082
4	-1.9011
5	-1.9010

It is not difficult to devise similar systematic procedures to perform Hulthén-Kohn variational calculations in more general cases. For example, if we consider the variational principle (10.25) for which the “normalization” (10.23) was adopted we may write the trial function  $u_l(r)$  as

$$u_l(r) = \phi_l(r) + \sum_{i=1}^N c_i \chi_i(r) \quad (10.36)$$

where  $\phi_l(r)$  yields the “asymptotic” part of  $u_l(r)$ , namely

$$\phi_l(r) \xrightarrow{r \rightarrow \infty} \sin(kr - \tfrac{1}{2}l\pi) + \lambda_l \cos(kr - \tfrac{1}{2}l\pi). \quad (10.37)$$

The variational parameters are  $c_i$  and  $\lambda_l$ , while the functions  $\chi_i(r)$  are some set of basis functions, confined to the region where the potential  $U(r)$  acts. For example

$$\chi_i(r) = e^{-\kappa r} r^i \quad (i = 1, 2, \dots, n) \quad (10.38)$$

where the additional nonlinear parameter  $\kappa$  is a scale factor which may also be varied.

With the choice of basis functions (10.38) and if eq. (10.37) is satisfied by the function  $\phi_l(r)$ , the trial function  $u_l(r)$  clearly obeys the boundary condition

(10.23) for  $r \rightarrow \infty$ . We recall, however, that we must also have  $u_l = 0$  at  $r = 0$ . Since the basis functions (10.38) are such that  $\chi_i(0) = 0$ , we must also impose the condition  $\phi_l(0) = 0$ . For example, in the case of s-wave scattering, we may write

$$\phi_0(r) = \sin kr + \lambda_0 \cos kr(1 - e^{-\kappa r}) \quad (10.39)$$

so that the trial function  $u_0(r)$  is then given explicitly by

$$u_0(r) = \sin kr + \lambda_0 \cos kr(1 - e^{-\kappa r}) + e^{-\kappa r} \sum_{i=1}^N c_i r^i. \quad (10.40)$$

Let us now return to the variational principle (10.25). For a *given* value of the nonlinear parameter  $\kappa$ , the problem reduces to a simple one of matrix inversion. Indeed, using eq. (10.36) and defining

$$\begin{aligned} A_{ij} &= A_{ji} = k^{-1} \int_0^\infty \chi_i L_i [\chi_j] dr \\ B_i &= k^{-1} \int_0^\infty \chi_i L_i [\phi_i] dr \\ C &= k^{-1} \int_0^\infty \phi_i L_i [\phi_i] dr \end{aligned} \quad (10.41)$$

the variational principle (10.25) reads

$$[\lambda_l] = \sum_{i=1}^N \sum_{j=1}^N c_i c_j A_{ij} + 2 \sum_{i=1}^N c_i B_i + C + \lambda_l. \quad (10.42)$$

Let us perform the variation with respect to the parameters  $c_i$ . This yields the system of  $N$  linear equations

$$\sum_{j=1}^N A_{ij} c_j = -B_i \quad (i = 1, 2, \dots, n) \quad (10.43)$$

so that, by inversion of the matrix  $(A_{ij})$ , one determines the variational parameters  $c_i$ . Varying also with respect to  $\lambda_l$  and substituting in eq. (10.42) one then obtains the stationary value  $[\lambda_l]$ , "second order accurate". The calculation may then be repeated for several values of the nonlinear parameter  $\kappa$ .

A similar procedure may of course be applied to the variational principle (10.31), with now

$$u^0(r) = \phi^0(r) + \sum_{i=1}^N c_i \chi_i(r) \quad (10.44)$$

and

$$\phi^0(r) \rightarrow \alpha - r. \quad (10.45)$$

Schwartz [15] has pointed out that the finite matrix  $(A_{ij})$  which represents the operator  $L_i$  in the space spanned by the  $N$  basis functions  $\chi_i$ , can occasionally have an eigenvalue very close to zero. In this case the whole variational procedure is meaningless. This fact can only occur because the variational principles discussed here, by contrast with those used in the study of bound

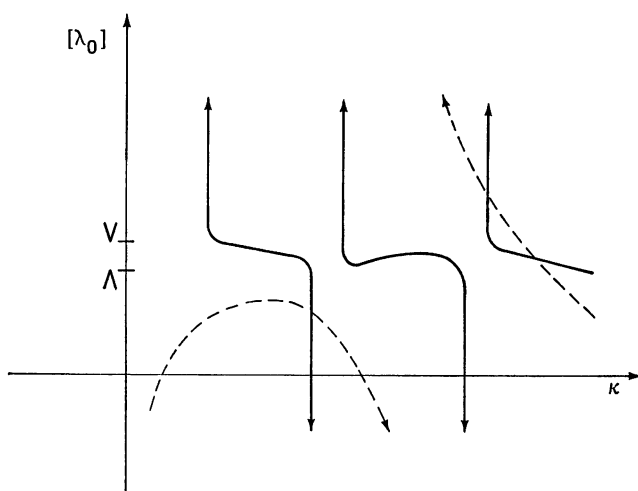


Fig. 10.1. Schematic plot of variational estimates of  $\lambda_0$  as a function of the non-linear parameter  $\kappa$ . For small values of  $N$  (the number of linear variational parameters) the singularities are broad and there are no flat regions (dashed curve). For  $N$  large (solid curve) there are more singularities but they are narrow and there are flat regions leading to the variational estimate of  $\lambda_0$  shown on the ordinate axis.

states, are not minimum principles but simply *stationary* principles. A typical variational calculation, where  $[\lambda_0]$  is shown as a function of the nonlinear parameter  $\kappa$  is displayed in Fig. 10.1. From this example, we see that the saving grace of the variational procedure is that the average value of  $[\lambda_0]$  between the singularities becomes smooth and flat. In this way a reasonably convergent extrapolation procedure can be devised and precise values of the phase shifts can be obtained. Several methods have also been proposed to avoid the difficulties connected with the appearance of these singularities [see e.g. 16].

The Hulthén-Kohn method has been extended to the calculation of phase shifts corresponding to the (low energy) scattering of a particle by a composite system including, if necessary, the effects of the Pauli exclusion principle between the incident and target particles. We shall examine this question in Chapter 19, where three-body problems are discussed.

### 10.1.2. Variational principle for the scattering amplitude

The Hulthén-Kohn variational principle can also be formulated for the scattering amplitude. In this case we start from the Schrödinger equation

$$[\nabla_{\mathbf{r}}^2 + k^2 - U(\mathbf{r})]\psi(\mathbf{r}) = 0 \quad (10.46)$$

and consider the integral

$$I[\psi_{-k_i}, \psi_{k_i}] = \int \psi_{-k_i}(\mathbf{r})[\nabla_{\mathbf{r}}^2 + k^2 - U(\mathbf{r})]\psi_{k_i}(\mathbf{r}) d\mathbf{r} \quad (10.47)$$

where the wave function  $\psi_{\mathbf{k}_i}(\mathbf{r})$  has the asymptotic form

$$\psi_{\mathbf{k}_i}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} [\exp(i\mathbf{k}_i \cdot \mathbf{r}) + f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}}) \exp(ikr)/r] \quad (10.48)$$

and  $\psi_{-\mathbf{k}_i}(\mathbf{r})$  has a similar asymptotic form with  $\mathbf{k}_i$  replaced by  $-\mathbf{k}_i$ . Introducing the variations  $\delta\psi_{\mathbf{k}_i}$  and  $\delta\psi_{-\mathbf{k}_i}$  such that

$$\delta\psi_{\mathbf{k}_i} \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \frac{e^{ikr}}{r} \delta f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}}) \quad (10.49)$$

and

$$\delta\psi_{-\mathbf{k}_i} \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \frac{e^{ikr}}{r} \delta f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}}) \quad (10.50)$$

one can show by using Green's theorem that [6]

$$\delta I = - (2\pi^2)^{-1} f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_i) \quad (10.51)$$

so that the functional

$$J \equiv I + (2\pi^2)^{-1} f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_i) \quad (10.52)$$

is stationary for variations of  $\psi_{\mathbf{k}_i}$  and  $\psi_{-\mathbf{k}_i}$  around their correct values. Since  $I = 0$  for the exact wave function, we obtain

$$[f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_i)] = f(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_i) + 2\pi^2 I[\psi_{-\mathbf{k}_i}, \psi_{\mathbf{k}_i}] \quad (10.53)$$

which is a direct extension of eq. (10.19). We note that for the simplest choice of trial functions, namely

$$\psi_{\mathbf{k}_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \quad (10.54)$$

and

$$\psi_{-\mathbf{k}_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \quad (10.55)$$

one has  $f = 0$  and

$$I = - (2\pi)^{-3} \int \exp\{i(\mathbf{k}_i - \mathbf{k}_i) \cdot \mathbf{r}\} U(\mathbf{r}) d\mathbf{r} \quad (10.56)$$

so that  $[f]$ , as given by eq. (10.53), reduces to the first Born approximation (8.26).

## 10.2. The Schwinger variational principle

### 10.2.1. Variational principle for the scattering amplitude

We begin by recalling the two integral representations of the scattering amplitude given by eqs. (5.40) and (5.74), namely

$$f = - 2\pi^2 \langle \Phi_{\mathbf{k}_i} | U | \psi_{\mathbf{k}_i}^{(+)} \rangle \quad (10.57)$$

and

$$f = - 2\pi^2 \langle \psi_{\mathbf{k}_i}^{(-)} | U | \Phi_{\mathbf{k}_i} \rangle. \quad (10.58)$$

Moreover, from the Lippmann-Schwinger equation (5.53) we also deduce that

$$|\Phi_{\mathbf{k}_i}\rangle = |\psi_{\mathbf{k}_i}^{(+)}\rangle - G_0^{(+)} U |\psi_{\mathbf{k}_i}^{(+)}\rangle \quad (10.59)$$

which, upon substitution into eq. (10.58) yields

$$f = -2\pi^2[\langle\psi_{k_t}^{(-)}|U|\psi_{k_1}^{(+)}\rangle - \langle\psi_{k_t}^{(-)}|UG_0^{(+)}U|\psi_{k_1}^{(+)}\rangle]. \quad (10.60)$$

After these preliminaries, we are now able to write down a variational principle for the scattering amplitude  $f$ . It is given by

$$[f] = -2\pi^2[\langle\Phi_{k_t}|U|\psi_{k_1}^{(+)}\rangle + \langle\psi_{k_t}^{(-)}|U|\Phi_{k_1}\rangle - \langle\psi_{k_t}^{(-)}|U - UG_0^{(+)}U|\psi_{k_1}^{(+)}\rangle]. \quad (10.61)$$

We first note from eqs. (10.57), (10.58) and (10.60) that the expression (10.61) is indeed a correct representation of the scattering amplitude. That is, it gives the *exact* scattering amplitude when the *exact* wave functions  $\psi_{k_1}^{(+)}$  and  $\psi_{k_t}^{(-)}$  are used.

Let us now verify that  $\delta[f] = 0$  for arbitrary variations of the bra  $\langle\psi_{k_t}^{(-)}|$  and the ket  $|\psi_{k_1}^{(+)}\rangle$  around their correct values. Varying first the bra  $\langle\psi_{k_t}^{(-)}|$  by an amount  $\langle\delta\psi_{k_t}^{(-)}|$ , we have

$$\delta[f] = -2\pi^2[\langle\delta\psi_{k_t}^{(-)}|U|\Phi_{k_1}\rangle - \langle\delta\psi_{k_t}^{(-)}|U - UG_0^{(+)}U|\psi_{k_1}^{(+)}\rangle]. \quad (10.62)$$

Therefore, if  $|\psi_{k_1}^{(+)}\rangle$  satisfies the Lippmann-Schwinger equation (5.53), we have

$$\delta[f] = 0. \quad (10.63)$$

Similarly, by varying the ket  $|\psi_{k_1}^{(+)}\rangle$  around its correct value, we find that eq. (10.63) is verified if the bra  $\langle\psi_{k_t}^{(-)}|$  satisfies the equation

$$\langle\psi_{k_t}^{(-)}| = \langle\Phi_{k_t}| + \langle\psi_{k_t}^{(-)}|UG_0^{(+)} \quad (10.64)$$

which is equivalent to eq. (5.65). The expression (10.61) which is bilinear in  $|\psi_{k_1}^{(+)}\rangle$  and  $\langle\psi_{k_t}^{(-)}|$  is called the *bilinear form of Schwinger's variational principle*.

We may at once take advantage of the variational principle (10.61) by choosing trial kets and bra's such that

$$|\psi_{k_1}^{(+)}\rangle \rightarrow A|\psi_{k_1}^{(+)}\rangle \quad (10.65)$$

$$\langle\psi_{k_t}^{(-)}| \rightarrow B\langle\psi_{k_t}^{(-)}|$$

where  $A$  and  $B$  are variational parameters. Inserting these expressions in the variational principle (10.61) and varying with respect to  $A$  and  $B$ , we obtain the *fractional form of Schwinger's variational principle*

$$[f] = -2\pi^2 \frac{\langle\psi_{k_t}^{(-)}|U|\Phi_{k_1}\rangle\langle\Phi_{k_t}|U|\psi_{k_1}^{(+)}\rangle}{\langle\psi_{k_t}^{(-)}|U - UG_0^{(+)}U|\psi_{k_1}^{(+)}\rangle}. \quad (10.66)$$

We note that this variational principle, as does the bilinear form (10.61), incorporates automatically the correct boundary conditions (i.e. does not require trial wave functions which satisfy the boundary conditions as in the case of the Hulthén-Kohn method), and uses only the trial wave functions

in the region where the interaction is non-vanishing. Furthermore, the fractional form (10.66) is independent of the “normalization” adopted for the trial functions.

As a first illustration of the variational principle (10.66), let us replace in this expression the unknown exact quantities  $|\psi_{k_1}^{(+)}\rangle$  and  $\langle\psi_{k_1}^{(-)}|$  by the corresponding Born free waves  $|\Phi_{k_1}\rangle$  and  $\langle\Phi_{k_1}|$ . That is,

$$|\psi_{k_1}^{(+)}\rangle \simeq |\Phi_{k_1}\rangle \quad (10.67)$$

and

$$\langle\psi_{k_1}^{(-)}| \simeq \langle\Phi_{k_1}|.$$

With this simple choice of trial functions, we find by using eqs. (8.15) and (8.16) that [17]

$$[f] = f_{B1} \left[ \frac{1}{1 - \bar{f}_{B2}/f_{B1}} \right]. \quad (10.68)$$

If the quantity  $x = |\bar{f}_{B2}/f_{B1}|$  is small, we may expand the expression (10.68) and obtain

$$[f] = f_{B1} + \bar{f}_{B2} + \cdots \quad (10.69)$$

which agrees with the Born series through second order in the interaction potential. The expression (10.68), which is based on a variational principle, often gives more accurate results than the second Born approximation. This, however, is not always the case since in general the variational principle (10.66) is not a *minimum* principle.

An evaluation of eq. (10.66) using the approximation (10.67) together with more elaborate choices has been carried out for  $^3S_1$  nucleon–nucleon scattering described by a Yukawa potential [18] or by an exponential or a gaussian potential [11]. The variational results turn out indeed to be more accurate than the second Born approximation. This statement, however, is meaningless at low energies, where the Born series does not converge. In fact, the first Born approximation may even give less inaccurate cross sections than the variational estimate based on the simple choice (10.67). Such examples illustrate the difficulties that may appear when poor trial functions are used in variational principles. Applications of the variational expression (10.68) to weaker interactions provide more satisfactory results [19].

As another application of the Schwinger variational principle (10.66), let us consider the case of a non-local separable potential  $\langle r|U|r'\rangle = \lambda u(r)u(r')$  [see eq. (5.149)]. A simple calculation shows that in this case, *for any choice of trial functions*

$$[f] = \bar{f} \quad (10.70)$$

where  $\bar{f}$  is the exact scattering amplitude.

### 10.2.2. Schwinger variational principles for the phase shifts

The variational expression (10.66) also provides a direct way of obtaining variational principles for the phase shifts. If we develop the trial functions

$\psi_{k_l}^{(+)}(r)$  and  $\psi_{k_l}^{(-)}(r)$  in spherical harmonics and consider the coefficients as variational parameters, we obtain the following stationary expression

$$\left[ \frac{\tan \eta_l}{k} \right] = \frac{\left[ \int_0^\infty j_l(kr)U(r)u_l(r)r \, dr \right]^2}{\int_0^\infty dr \int_0^\infty dr' u_l(r)U(r)G_l(r, r')U(r')u_l(r')rr' - \int_0^\infty U(r)u_l^2(r) \, dr} \quad (10.71)$$

where

$$G_l(r, r') = kj_l(kr_<)n_l(kr_>) \quad (10.72)$$

while  $r_<$  and  $r_>$  and respectively the smaller and the larger of  $r$  and  $r'$ . Of course, one can directly establish the variational principle (10.71) by starting from the integral equation satisfied by the exact function  $\bar{u}_l(r)$ , namely [see eq. (5.98)]

$$\bar{u}_l(r) = rj_l(kr) + r \int_0^\infty G_l(r, r')U(r')\bar{u}_l(r')r' \, dr' \quad (10.73)$$

and using the relation [see eq. (5.96)]

$$\tan \bar{\eta}_l = -k \int_0^\infty j_l(kr)U(r)\bar{u}_l(r)r \, dr. \quad (10.74)$$

The foregoing treatment [5, 8] in fact historically preceded the variational principle (10.66) for the transition amplitude. It played an important role in nuclear theory where it allowed the first rigorous derivation of the effective range formulae [20] used in the analysis of low-energy nucleon-nucleon scattering. We also note that a *bilinear form* of the Schwinger variational principle for phase shifts may be written down by starting from the variational expression (10.61). It is given by

$$\left[ \frac{\tan \eta_l}{k} \right] = -2 \int_0^\infty j_l(kr)U(r)u_l(r)r \, dr + \int_0^\infty U(r)u_l^2(r) \, dr - \int_0^\infty dr \int_0^\infty dr' u_l(r)U(r)G_l(r, r')U(r')u_l(r')rr' \quad (10.75)$$

with

$$u_l(r) \xrightarrow{r \rightarrow \infty} rj_l(kr) - rn_l(kr) \tan \eta_l. \quad (10.76)$$

By analogy with the discussion of the Schwinger variational principle for the scattering amplitude we note that by choosing the simple trial function

$$u_l(r) = rj_l(kr) \quad (10.77)$$

and substituting in the stationary expression (10.71), we get

$$\left[ \frac{\tan \eta_l}{k} \right] = \frac{\left[ \int_0^\infty j_l^2(kr)U(r)r^2 dr \right]^2}{\int_0^\infty dr \int_0^\infty dr' j_l(kr)U(r)G_l(r, r')U(r')j_l(kr)r^2r'^2 - \int_0^\infty j_l^2(kr)U(r)r^2 dr} \quad (10.78)$$



which agrees with the Born series through second order [see eqs. (8.74)–(8.75)]. Again, this expression which rests on a variational principle is often more accurate than the second Born approximation.

As an example, let us compare various calculations of the scattering length  $\alpha$  corresponding to the square well (4.141) of depth  $U_0(>0)$  and of range  $a$ . Defining the dimensionless quantity

$$\beta = U_0^{1/2}a \quad (10.79)$$

the exact scattering length is given by eq. (4.157), namely

$$\bar{\alpha} = \left(1 - \frac{\tan \beta}{\beta}\right)a. \quad (10.80)$$

Note that  $\bar{\alpha}$  becomes infinite and changes sign at  $\beta = \frac{1}{2}\pi, \frac{3}{2}\pi$ , etc. The first Born approximation gives

$$\alpha_{B1} = -\frac{1}{3}\beta^2a \quad (10.81)$$

while the second Born approximation yields

$$\alpha_{B2} = -\left(\frac{1}{3}\beta^2 + \frac{2}{15}\beta^4\right)a. \quad (10.82)$$

With a simple trial function  $u^0(r) = r$  for zero-energy s-wave scattering, the Schwinger variational principle (10.71) leads to the result

$$[\alpha] = -\frac{1}{3}\beta^2a/(1 - \frac{2}{3}\beta^2). \quad (10.83)$$

These various expressions are compared in Table 10.3 where it is seen that the variational expression is very accurate. We note in particular that by expanding the quantities  $\bar{\alpha}$  and  $[\alpha]$  in powers of  $\beta^2$  (i.e. in powers of the

TABLE 10.3

Comparison of various calculations for the scattering length  $\alpha$ , as a function of  $\beta = U_0^{1/2}a$ . The values of  $\alpha$  are given in units of  $a$ . The numbers in parentheses indicate powers of 10.

$\beta$	$\alpha_{B1}$	$\alpha_{B2}$	$[\alpha]$	$\bar{\alpha}$
0	0	0	0	0
0.2	-1.33 (-2)	-1.35 (-2)	-1.36 (-2)	-1.36 (-2)
0.4	-5.33 (-2)	-5.67 (-2)	-5.70 (-2)	-5.70 (-2)
0.6	-1.20 (-1)	-1.37 (-1)	-1.40 (-1)	-1.40 (-1)
0.8	-2.13 (-1)	-2.68 (-1)	-2.87 (-1)	-2.87 (-1)
1.0	-3.33 (-1)	-4.67 (-1)	-5.56 (-1)	-5.57 (-1)
1.2	-4.80 (-1)	-7.56 (-1)	-1.13	-1.14
1.4	-6.53 (-1)	-1.17	-3.02	-3.14
1.6	-8.53 (-1)	-1.73	3.56 (+1)	2.24 (+1)
1.8	-1.08	-2.48	3.65	3.38
2.0	-1.33	-3.47	2.22	2.09
2.2	-1.61	-4.74	1.72	1.62
2.4	-1.92	-6.34	1.47	1.38
2.6	-2.25	-8.35	1.32	1.23
2.8	-2.61	-1.08 (+1)	1.22	1.13
3.0	-3.00	-1.38 (+1)	1.15	1.05

potential strength  $U_0$ ), we have from eq. (10.80)

$$\bar{\alpha} = -(\frac{1}{3}\beta^2 + \frac{2}{15}\beta^4 + 0.0533\beta^6 + \dots)a \quad (10.84)$$

while eq. (10.83) yields

$$[\alpha] = -(\frac{1}{3}\beta^2 + \frac{2}{15}\beta^4 + 0.0540\beta^6 + \dots)a. \quad (10.85)$$

Although the Schwinger variational principles are intrinsically superior to the corresponding differential variational principles, this advantage is usually offset by the fact that the matrix elements involving Green's functions which appear in Schwinger's method are tedious to evaluate in all but the simple cases. The greater simplicity of the Hulthén-Kohn forms, on the other hand, allows for the use of more elaborate trial functions, even for relatively complicated problems [see e.g. 15, 21].

### 10.3. Minimum principles in scattering theory

The scattering variational principles which we have developed thus far are stationary principles but they are not, in general, minimum (or maximum) principles. This fact constitutes an important difference when compared to bound state problems, where upper bounds on the energy eigenvalues are readily obtainable. Thus, in scattering problems the variational result can fall either above or below the true value. Without a minimum (maximum) principle, the variational determination of the parameters is only the most plausible one (in the absence of other information) and greater flexibility in the choice of trial functions may even lead to less satisfactory results. Therefore, in applying the variational principles discussed in the two preceding sections, great care must be taken and extensive work has in general to be done in order to obtain reliable results.

It is thus of considerable interest to develop variational principles giving upper and (or) lower bounds for phase shifts, scattering lengths, scattering amplitudes, etc. This was initiated by Kato [22] and developed extensively by various authors [see e.g. 23, 24]. As an introduction to these techniques, we shall derive in this section the Kato identity, and then limit our discussion to the case of variational bounds for scattering lengths.

#### 10.3.1. The Kato identity

Let us start from equation (10.4) and adopt for  $\bar{u}_l$  the "normalization" [25]

$$\bar{u}_l(r) \xrightarrow{r \rightarrow \infty} \cos(kr - \frac{1}{2}l\pi + \gamma) + \cot(\bar{\eta}_l - \gamma) \sin(kr - \frac{1}{2}l\pi + \gamma) \quad (10.86)$$

where  $\gamma$  is a fixed constant such that  $0 \leq \gamma < \pi$ . The trial function  $u_l(r)$  has the same asymptotic behaviour with  $\bar{\eta}_l$  replaced by  $\eta_l$ .

Now let us apply Green's theorem

$$\int_0^\infty \{f L_l[g] - g L_l[f]\} dr = \left[ f \frac{dg}{dr} - g \frac{df}{dr} \right]_0^\infty \quad (10.87)$$

where  $f = \bar{u}_l$  and  $g = u_l$ . Recalling that  $\bar{u}_l(0) = u_l(0) = 0$  and taking into account eq. (10.86), we get

$$\int_0^\infty \bar{u}_l L_l[u_l] dr = k \cot(\eta_l - \gamma) - k \cot(\bar{\eta}_l - \gamma). \quad (10.88)$$

Setting

$$w_l(r) = u_l(r) - \bar{u}_l(r) \quad (10.89)$$

and noting that

$$L_l[w_l] = L_l[u_l] \quad (10.90)$$

we obtain the *Kato identity*

$$k \cot(\bar{\eta}_l - \gamma) = k \cot(\eta_l - \gamma) - \int_0^\infty u_l L_l[u_l] dr + \int_0^\infty w_l L_l[w_l] dr. \quad (10.91)$$

The first two terms on the right-hand side of eq. (10.91) can be calculated by specifying the trial function  $u_l$ . They give an approximate value of the quantity  $k \cot(\bar{\eta}_l - \gamma)$ , while the last term (of order  $w_l^2$ ) should be small if  $u_l$  is a good approximation to  $\bar{u}_l$ . In fact, for the choice  $\gamma = \frac{1}{2}\pi$ , the neglect of the last term on the right side of eq. (10.91) leads to

$$[k \tan \eta_l] = k \tan \eta_l + \int_0^\infty u_l L_l[u_l] dr \quad (10.92)$$

which is precisely the Hulthén–Kohn variational principle (10.25). The above discussion can be generalized to elastic scattering by compound systems. A generalized version of the Kato identity can also be obtained for multichannel scattering.

Since eq. (10.91) is an exact formula, one may obtain bounds on  $k \cot(\bar{\eta}_l - \gamma)$  and, hence, on  $\bar{\eta}_l$ , if the last term on the right of equation (10.91) can be estimated. We illustrate this point in the next paragraph by showing how *variational bounds* can be obtained for *scattering lengths*.

#### 10.4.2. Variational bounds for scattering lengths

Let us consider the simple case of s-wave scattering by a short-range potential at zero incident energy [26]. Choosing  $\gamma = \frac{1}{2}\pi$  in eq. (10.91) we have (with  $L_0 \equiv L$ )

$$\bar{\alpha} = \alpha - \int_0^\infty u^0 L[u^0] dr + \int_0^\infty w L[w] dr \quad (10.93)$$

where  $\bar{\alpha}$  and  $\alpha$  denote, respectively, the exact and trial scattering lengths while the radial functions  $\bar{u}^0(r)$  and  $u^0(r)$  corresponding to zero energy s-wave scattering are such that

$$\bar{u}^0(0) = u^0(0) = 0 \quad (10.94)$$

$$\bar{u}^0(r) \xrightarrow{r \rightarrow \infty} \bar{\alpha} - r \quad (10.95)$$

and

$$u^0(r) \xrightarrow{r \rightarrow \infty} \alpha - r. \quad (10.96)$$

We note that the function  $w = u^0 - \bar{u}^0$  satisfies the boundary conditions

$$w(0) = 0 \quad (10.97)$$

and

$$w(r) \xrightarrow{r \rightarrow \infty} \alpha - \bar{\alpha}. \quad (10.98)$$

Now, if the potential cannot support a bound state, one has

$$\int_0^\infty wL[w] \, dr \leq 0. \quad (10.99)$$

To prove this statement, we first note that if no bound state exists,  $L$  is a negative definite operator on the space of quadratically integrable functions. This argument, however, cannot be applied directly to the case considered here since the function  $w(r)$  approaches a constant value for large  $r$  and is therefore not quadratically integrable. Nevertheless, if we introduce the functions

$$w_\lambda(r) \equiv w(r) e^{-\lambda r} \quad (10.100)$$

with  $\lambda > 0$ , we have

$$M(\lambda) \equiv \int_0^\infty w_\lambda(r) L[w_\lambda(r)] \, dr \leq 0. \quad (10.101)$$

To show that  $M(0)$  is not positive, it remains to prove that  $M(\lambda)$  is continuous at  $\lambda = 0$ . This is easily done by considering the quantity

$$\begin{aligned} M(\lambda) - M(0) &= \int_0^\infty w(r) [e^{-2\lambda r} - 1] L[w(r)] \, dr \\ &\quad + \lambda^2 \int_0^\infty w^2(r) e^{-2\lambda r} \, dr - 2\lambda \int_0^\infty w(r) w'(r) e^{-2\lambda r} \, dr \end{aligned} \quad (10.102)$$

and checking that each of the three terms on the right-hand side of eq. (10.102) vanishes in the limit  $\lambda \rightarrow 0$ . Thus, if no bound state exists, the scattering length satisfies the relation

$$\bar{\alpha} \leq [\alpha] = \alpha - \int_0^\infty u^0 L[u^0] \, dr \quad (10.103)$$

with

$$u^0(0) = 0 \quad (10.104)$$

and

$$u^0(r) \xrightarrow{r \rightarrow \infty} \alpha - r. \quad (10.105)$$

We recognize on the right-hand side of eq. (10.103) the Hulthén-Kohn variational principle (10.31) for the scattering length, which therefore gives

an upper bound on  $\bar{\alpha}$  under the above specified conditions. The procedure to determine the variational parameters is now perfectly unambiguous. Using a trial function  $u^0(c_1, c_2, \dots, c_n; \alpha; r)$  one determines the variational parameters  $c_1, c_2, \dots, c_n$  and  $\alpha$  by solving the system of equations

$$\frac{\partial[\alpha]}{\partial c_i} = 0 \quad (i = 1, 2, \dots, n) \quad (10.106)$$

and

$$\partial[\alpha]/\partial\alpha = 0. \quad (10.107)$$

For linear variational parameters, this system leads to a unique set of values for the parameters. For nonlinear variational parameters, there is in general more than one set of parameters. In this case eq. (10.103) shows that one should choose the set which gives the lowest value of  $[\alpha]$ .

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# Analytic Properties of Scattering Amplitudes

Since the early work of Kramers, Møller and Heisenberg [1–3] who first related bound states to analytic properties of scattering amplitudes, the study of these amplitudes as functions of complex energies, complex wave numbers and even complex angular momenta has been developed in great detail.

We shall present in this chapter an introduction to these methods within the framework of non-relativistic scattering by a central potential, where the basic ideas of this approach can be illustrated in a simple way. The full scope and utility of these techniques, however, is only apparent in more complicated situations, particularly in “elementary particle” physics [see e.g. 4].

We begin in Section 11.1 by introducing the Jost functions [5] and studying their analytic properties. The properties of the  $S$ -matrix elements and the partial wave amplitudes as functions of complex wave numbers and complex energies are then investigated in Section 11.2. An important theorem due to Levinson [6], which relates the zero-energy value of the phase shift to the number of bound states, is proved in Section 11.3. The next section is devoted to the study of Regge poles [7] which arise in the investigation of the analytic properties of the  $S$ -matrix in the complex angular momentum plane. Dispersion relations are considered in Section 11.5. Finally, in Section 11.6 we make use of the analytic properties of scattering amplitudes to examine low energy potential scattering and derive the effective range theory.

## 11.1. The Jost functions

Let us consider s-wave ( $l = 0$ ) scattering by a central potential. The radial Schrödinger equation reads

$$[d^2/dr^2 + k^2 - U(r)]u(k, r) = 0 \quad (11.1)$$

where we have dropped the subscript referring to  $l = 0$  and exposed explicitly the dependence of the function  $u$  on the wave number  $k$ .

We shall assume that the reduced potential  $U(r)$  is less singular than  $r^{-2}$  at the origin and vanishes faster than  $r^{-3}$  at infinity. Thus

$$\int_0^{\infty} dr \, r |U(r)| < \infty \quad (11.2)$$

and

$$\int_0^{\infty} dr \, r^2 |U(r)| < \infty. \quad (11.3)$$

The point  $r = 0$  is therefore a regular point of the differential equation (11.1). The solutions of eq. (11.1) which vanish at the origin are generally called *regular*; those which do not are *irregular*. The physical solution  $u(k, r)$  introduced in Chapter 4, satisfies the boundary conditions

$$u(k, 0) = 0, \quad (11.4a)$$

$$u(k, r) \xrightarrow{r \rightarrow \infty} A \sin(kr + \delta) \quad (11.4b)$$

and is evidently a regular solution. Another interesting regular solution  $\phi(k, r)$  of eq. (11.1) is defined by the simple conditions at  $r = 0$

$$\phi(k, 0) = 0 \quad (11.5a)$$

and

$$\phi'(k, 0) = 1 \quad (11.5b)$$

where the prime denotes differentiation with respect to  $r$ . We may also write that the function  $\phi(k, r)$  satisfies the boundary condition

$$\lim_{r \rightarrow 0} r^{-1} \phi(k, r) = 1. \quad (11.6)$$

The conditions (11.5) have several interesting implications. First of all, the function  $\phi(k, r)$  must be *real* for real  $k$ . Secondly, since eq. (11.1) depends only on  $k$  through  $k^2$  and the conditions (11.5)–(11.6) are independent of  $k$ , the function  $\phi(k, r)$  is an *even* function of  $k$ ,

$$\phi(-k, r) = \phi(k, r). \quad (11.7)$$

Finally, as a consequence of a theorem proved by Poincaré [8], the absence of  $k$  dependence in the boundary conditions (11.5) implies that  $\phi(k, r)$ , considered as a function of  $k$ , is an *entire* function of  $k$ . That is,  $\phi(k, r)$  is an *analytic* function of  $k$  in the *open* complex  $k$ -plane.

Since the function  $\phi(k, r)$  is real for real  $k$ , we can use the Schwarz reflection principle [9] to deduce that

$$\phi^*(k^*, r) = \phi(k, r). \quad (11.8)$$

Let us now consider two *irregular* solutions  $f(\pm k, r)$  of eq. (11.1) which we define by the relations

$$\lim_{r \rightarrow \infty} e^{\pm ikr} f(\pm k, r) = 1. \quad (11.9)$$



The boundary conditions (11.9) do not define  $f(k, r)$  in the upper half complex  $k$ -plane or  $f(-k, r)$  in the lower half  $k$ -plane. However, we shall now prove that, if the inequalities (11.2) and (11.3) are satisfied,  $f(k, r)$  is, for all  $r$ , an *analytic* function of  $k$  when  $\text{Im } k < 0$  while  $f(-k, r)$  is, for all  $r$ , an analytic function of  $k$  if  $\text{Im } k > 0$ .

Let us first consider the function  $f(k, r)$ . Following Bargmann [10], we set

$$g(k, r) = e^{ikr} f(k, r). \quad (11.10)$$

Then

$$[d^2/dr^2 - 2ik \, d/dr]g(k, r) = U(r)g(k, r) \quad (11.11)$$

and

$$\lim_{r \rightarrow \infty} g(k, r) = 1 \quad (11.12)$$

for every real non-vanishing  $k$ . We now replace eqs. (11.11) and (11.12) by the Volterra integral equation

$$g(k, r) = 1 + \int_r^\infty D_k(r' - r)U(r')g(k, r') \, dr' \quad (11.13)$$

where

$$D_k(\xi) = \frac{1 - e^{-2ik\xi}}{2ik} = \int_0^\xi e^{-2ikx} \, dx. \quad (11.14)$$

We readily verify that a solution of the integral equation (11.13) satisfies eqs. (11.11)–(11.12) provided uniform convergence in  $r$  allows one to differentiate under the integral sign. We now attempt to solve eq. (11.13) by the series

$$g(k, r) = \sum_{n=0}^\infty g_n(k, r) \quad (11.15)$$

where

$$g_0(k, r) = 1 \quad (11.16)$$

and

$$g_n(k, r) = \int_r^\infty D_k(r' - r)U(r')g_{n-1}(k, r') \, dr'. \quad (11.17)$$

We shall prove that the series (11.15) converges when  $\text{Im } k < 0$ . We assume that the inequality (11.2) is true and set

$$X(r) = \int_r^\infty r' |U(r')| \, dr'. \quad (11.18)$$

If  $\text{Im } k < 0$ , then we may use eq. (11.14) to write

$$|D_k(r' - r)| \leq r' - r \leq r' \quad (11.19)$$

and by induction

$$|g_n(k, r)| \leq \frac{[X(r)]^n}{n!} \leq \frac{[X(0)]^n}{n!}. \quad (11.20)$$

Therefore the series (11.15) converges towards a solution. Differentiating the series with respect to  $k$  we also obtain by the same reasoning a convergent series because of the inequality (11.3). Hence the function  $f(k, r)$  exists and is analytic in the lower-half  $k$ -plane. In the same way  $f(-k, r)$  can be shown to be analytic in the upper-half  $k$ -plane.

We may extend the region of analyticity of the functions  $f(\pm k, r)$  if we impose stronger conditions on the potential. Thus, if we assume that

$$I(\mu) = \int_0^\infty e^{\mu r} |U(r)| dr < \infty, \quad \mu \text{ real} > 0 \quad (11.21)$$

then  $f(k, r)$  is analytic for  $\text{Im } k < \frac{1}{2}\mu$  and  $f(-k, r)$  is analytic for  $\text{Im } k > -\frac{1}{2}\mu$  (see Fig. 11.1).

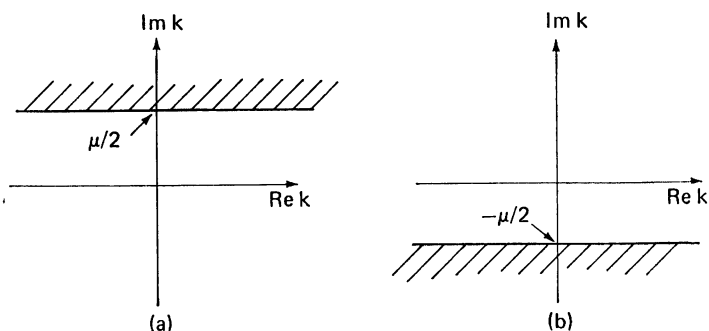


Fig. 11.1. The unshaded areas are the regions of analyticity (a) of  $f(k, r)$ ; (b) of  $f(-k, r)$  when the condition (11.21) is satisfied by the potential.

To prove these statements, we assume that  $\text{Im } k \leq \frac{1}{2}\mu_1$  with  $\mu_1 < \mu$ . We note that

$$|D_k(\xi)| \leq \xi \exp(\mu_1 \xi) \leq C \exp(\mu \xi) \quad (11.22)$$

where  $C$  is a suitably chosen constant. Defining

$$Y(r) = \int_r^\infty \exp(\mu r') |U(r')| dr' \quad (11.23)$$

we find by induction that

$$|g_n(k, r)| \leq [CY(r)]^n/n! \leq [CI(\mu)]^n/n! \quad (11.24)$$

which proves the uniform convergence of the series (11.15). The analyticity of  $g(k, r)$  and therefore of  $f(k, r)$  is obtained by differentiating with respect to  $k$  and using the same arguments. The analytic character of  $f(-k, r)$  for  $\text{Im } k > -\frac{1}{2}\mu$  clearly follows in a completely analogous way.

Finally, if the potential has a strict finite range (i.e. vanishes identically beyond a certain distance  $a$ ), then  $I(\mu)$  is finite for all  $\mu$ , so that  $f(k, r)$  and  $f(-k, r)$  are *entire* analytic functions of  $k$ . It is worth noting that the existence of singularities in the functions  $f(\pm k, r)$  is very sensitive to the tail of the potential. If we cut the potential  $U(r)$  at a distance  $r = a$ , even arbitrarily large, all the singularities of  $f(\pm k, r)$  disappear.

Let us now relate the two functions  $f(k, r)$  and  $f(-k, r)$ . If the condition (11.21) holds, we deduce from eq. (11.9) that in a region of analyticity connected to the real axis

$$f^*(-k^*, r) = f(k, r). \quad (11.25)$$

Next, we relate the two irregular solutions  $f(\pm k, r)$  to the regular solution  $\phi(k, r)$ . Since the solutions  $f(k, r)$  and  $f(-k, r)$  are clearly linearly independent – except for  $k = 0$  – we may express  $\phi(k, r)$  in terms of  $f(\pm k, r)$ . Let us write

$$\phi(k, r) = a(k)f(-k, r) + b(k)f(k, r). \quad (11.26)$$

The coefficients  $a(k)$  and  $b(k)$  are easily obtained by evaluating the Wronskians [11]  $W[f(k, r), \phi(k, r)]$  and  $W[f(-k, r), \phi(k, r)]$ . Thus

$$W[f(k, r), \phi(k, r)] = a(k)W[f(k, r), f(-k, r)] \quad (11.27)$$

and

$$W[f(-k, r), \phi(k, r)] = b(k)W[f(-k, r), f(k, r)]. \quad (11.28)$$

Since the Wronskian of two linearly independent solutions is independent of  $r$ , we may evaluate  $W[f(-k, r), f(k, r)]$  in the limit  $r \rightarrow \infty$ . Then, by using eq. (11.9), we find that

$$W[f(k, r), f(-k, r)] = 2ik. \quad (11.29)$$

We now define the *Jost functions*  $\mathcal{J}(\pm k)$  such that

$$\mathcal{J}(\pm k) = W[f(\pm k, r), \phi(k, r)] \quad (11.30)$$

and therefore

$$\phi(k, r) = \frac{1}{2ik} [\mathcal{J}(k)f(-k, r) - \mathcal{J}(-k)f(k, r)]. \quad (11.31)$$

Furthermore, if we evaluate the Wronskian of eq. (11.30) at  $r = 0$  and use eqs. (11.5) and (11.6), we find that

$$\mathcal{J}(\pm k) = f(\pm k, 0). \quad (11.32)$$

The Jost functions  $\mathcal{J}(\pm k)$  clearly enjoy the same analyticity properties as the functions  $f(\pm k, r)$ . Also, from eq. (11.25), we find that

$$\mathcal{J}^*(-k^*) = \mathcal{J}(k) \quad (11.33)$$

while eqs. (11.10), (11.13) and (11.32) may be used to derive an integral representation of  $\mathcal{J}(k)$ , namely

$$\mathcal{J}(k) = 1 + \int_0^\infty D_k(r)U(r) e^{ikr} f(k, r) dr. \quad (11.34)$$

From this equation we deduce that  $\mathcal{J}(k) \rightarrow 1$  as  $|k| \rightarrow \infty$  and  $\text{Im } k \leq 0$ .

We now prove a very important property of the Jost function  $\mathcal{J}(k)$ , namely that *its zeros in the lower half  $k$ -plane correspond to bound states*. Indeed, let

us assume that  $\mathcal{J}(k) = 0$  for  $k = k_0$ . Since  $\mathcal{J}(k) = W[f(k, r), \phi(k, r)]$ , we have

$$W[f(k_0, r), \phi(k_0, r)] = 0 \quad (11.35)$$

and  $f(k_0, r)$  is therefore a multiple of  $\phi(k_0, r)$ , i.e.

$$f(k_0, r) = C\phi(k_0, r); \quad C = \text{const.} \quad (11.36)$$

Since the left-hand side of eq. (11.36) behaves for large  $r$  as  $\exp(-ik_0 r)$ , and  $\phi(k, r)$  vanishes at  $r = 0$ , we see that  $\phi(k_0, r)$  is a square integrable eigenfunction of the Schrödinger equation corresponding to the eigenvalue  $k_0^2$ , provided  $\text{Im } k_0 < 0$ . It is also a simple matter to show that  $\text{Re } k_0 = 0$  so that the corresponding bound state energy  $E = \hbar^2 k_0^2 / 2m$  is indeed real and negative.

Furthermore, if the point  $-k_0 = i|k_0|$  lies within a region to which  $f(k, r)$  can be analytically continued we may calculate the constant  $C$  from eq. (11.31), i.e.

$$C = -\frac{2|k_0|}{\mathcal{J}(i|k_0|)} \quad (11.37)$$

so that

$$\lim_{r \rightarrow \infty} \phi(-i|k_0|, r) = C^{-1} \exp(-|k_0|r). \quad (11.38)$$

It is worth noting that the Jost function  $\mathcal{J}(k)$  cannot vanish for  $k$  real  $\neq 0$ . Otherwise we would also have  $\mathcal{J}(-k) = 0$  and therefore  $\phi(k, r) = 0$  [see eq. (11.31)], in contradiction with the boundary condition (11.6). The point  $k = 0$  is therefore the only one on the real  $k$ -axis where the Jost function may vanish. However, in contrast with the case  $\text{Im } k < 0$ , the fact that  $\mathcal{J}(0) = 0$  does not imply a bound state [12]. Indeed, from eq. (11.36) we see that

$$f(0, r) = C\phi(0, r). \quad (11.39)$$

Since  $f(0, r) \rightarrow 1$  for  $r \rightarrow \infty$ , the function  $\phi(0, r)$  is not square integrable, so that a zero of  $\mathcal{J}(k)$  at  $k = 0$  does not correspond to a bound state [13]. Furthermore, if  $k$  approaches zero from the lower half-plane, it can be shown [14] that  $\mathcal{J}(k)$  tends to zero as  $k$ , i.e.

$$\mathcal{J}(k) \sim \mathcal{O}(k); \quad [\mathcal{J}(k)]^{-1} \sim \mathcal{O}(k^{-1}). \quad (11.40)$$

We now prove that the zeros of the Jost function at the points  $k_0 = -i|k_0|$  are simple [15]. We first note that the Wronskian of two solutions  $f_1(k, r)$  and  $f_2(k', r)$  of the radial Schrödinger equation (11.1) corresponding to different wave numbers  $k$  and  $k'$  satisfies the equation

$$\frac{\partial}{\partial r} W[f_1(k, r), f_2(k', r)] = (k^2 - k'^2)f_1(k, r)f_2(k', r) \quad (11.41)$$

so that

$$W[\phi(k, r), \phi(k_0, r)] = (k^2 - k_0^2) \int_0^r dr' \phi(k, r')\phi(k_0, r') \quad (11.42a)$$

and

$$W[f(k, r), f(k_0, r)] = -(k^2 - k_0^2) \int_r^\infty dr' f(k, r') f'(k_0, r'). \quad (11.42b)$$

Next we differentiate eq. (11.30) with respect to  $k^2$  (indicated by a dot), set  $k = k_0$  and use eq. (11.36) to obtain

$$\begin{aligned} \not{J}(k_0) &= W[\dot{f}(k_0, r), \phi(k_0, r)] + W[f(k_0, r), \dot{\phi}(k_0, r)] \\ &= C^{-1} W[\dot{f}(k_0, r), f(k_0, r)] + C W[\phi(k_0, r), \dot{\phi}(k_0, r)]. \end{aligned} \quad (11.43)$$

If we now differentiate eqs. (11.42) with respect to  $k^2$  and use the results in eq. (11.43), we find that

$$[\partial \not{J} / \partial k^2]_{k=k_0} = -C \int_0^\infty \phi^2(k_0, r) dr. \quad (11.44)$$

Since  $\phi(k_0, r)$  is real and  $C$  cannot vanish – otherwise the boundary condition (11.9) would be violated – we see that

$$[\partial \not{J} / \partial k]_{k=k_0} = -2k_0 C \int_0^\infty \phi^2(k_0, r) dr \neq 0 \quad (11.45)$$

and therefore the zeros of  $\not{J}(k)$  in the lower half  $k$ -plane are simple. This shows that the radial Schrödinger equation (11.1) for  $l = 0$  cannot have degenerate eigenvalues. Only for other values of  $l$  can degeneracies arise.

The zeros of  $\not{J}(k)$  in the upper half-plane [or those of  $\not{J}(-k)$  in the lower half plane] do not have the same meaning since in this case  $f(k, r)$  [or  $f(-k, r)$ ] grows exponentially with  $r$  at large distances. In fact these zeros are not confined to the imaginary axis but because of eq. (11.33) they appear in symmetrical pairs about the imaginary axis (see Fig. 11.2).

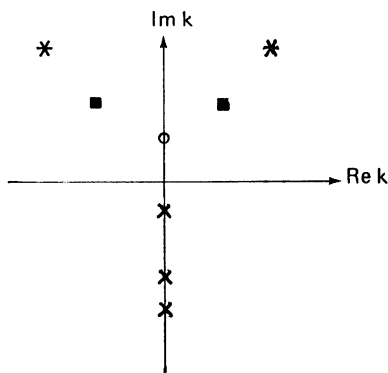


Fig. 11.2. The zeros of the Jost function  $\not{J}(k)$ .  $\times$ : Zeros appearing on the negative imaginary axis and corresponding to bound states.  $\blacksquare$ ,  $*$ : Zeros appearing by pairs in the upper half plane, and symmetrical about the imaginary axis.  $\circ$ : Possible zeros on the positive imaginary axis.

The above analysis of the properties of the Jost functions may be extended to higher angular momenta ( $l \geq 1$ ); a detailed discussion may be found in the work of Newton [14]. Starting from the radial equation (4.17), namely

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - U(r)]u_l(k, r) = 0 \quad (11.46)$$

we now define regular solutions  $\phi_l(k, r)$  of this equation, such that

$$\lim_{r \rightarrow 0} r^{-l-1} \phi_l(k, r) = 1. \quad (11.47)$$

As a consequence of the Poincaré theorem mentioned above the functions  $\phi_l(k, r)$  are *entire* functions of  $k$ .

Irregular solutions  $f_l(\pm k, r)$  of eq. (11.46) may still be defined by the boundary condition (11.9), namely

$$\lim_{r \rightarrow \infty} e^{\pm ikr} f_l(\pm k, r) = 1. \quad (11.48)$$

The analytic properties of  $f_l(\pm k, r)$  in the complex  $k$ -plane are identical to those already discussed for the case  $l = 0$ , except at  $k = 0$ . Thus  $f_l(k, r)$  is analytic in the lower half  $k$ -plane if the potential satisfies the conditions (11.2) and (11.3), except at  $k = 0$  where it has a pole of order  $l$ . If the more stringent inequality (11.21) is true, the domain of analyticity of  $f_l(k, r)$  may be extended in the upper half-plane to  $\text{Im } k < \frac{1}{2}\mu$ . If the potential has a strict finite range, the function  $f_l(k, r)$  is analytic in the open  $k$ -plane, except at  $k = 0$ .

The corresponding "generalized" Jost functions  $\tilde{f}_l(k)$  are defined by the extension of eq. (11.30), namely

$$\tilde{f}_l(\pm k) = W[f_l(\pm k, r), \phi_l(k, r)] \quad (11.49)$$

so that

$$\phi_l(k, r) = \frac{1}{2ik} [\tilde{f}_l(k) f_l(-k, r) - \tilde{f}_l(-k) f_l(k, r)]. \quad (11.50)$$

Furthermore, if the condition (11.21) holds, we may write

$$\tilde{f}_l^*(-k^*) = \tilde{f}_l(k). \quad (11.51)$$

We note, however, that the simple relation (11.32) is no more true in this case; we have instead

$$\tilde{f}_l(\pm k) = (2l+1) \lim_{r \rightarrow 0} r^l f_l(\pm k, r). \quad (11.52)$$

Moreover, one has now

$$\lim_{|k| \rightarrow \infty} k^l \tilde{f}_l(\pm k) = (2l+1)!! \exp(\mp \frac{1}{2}i\pi) \quad (11.53)$$

with  $\text{Im } k \leq 0$  for the function  $\tilde{f}_l(+k)$  and  $\text{Im } k \geq 0$  for  $\tilde{f}_l(-k)$ , respectively. It is therefore convenient to introduce other Jost functions  $f_l(\pm k)$  such that

$$f_l(\pm k) = \frac{k^l \exp(\pm \frac{1}{2}i\pi)}{(2l+1)!!} \tilde{f}_l(\pm k) \quad (11.54)$$

which are continuous at  $k = 0$  and such that  $f_l(\pm k) \rightarrow 1$  as  $|k| \rightarrow \infty$  (with  $\text{Im } k \leq 0$  or  $\text{Im } k \geq 0$ , respectively). The Jost functions  $f_l(\pm k)$  also satisfy eq. (11.51). The study of their analytic properties is similar to that made for the case  $l = 0$ , except that a zero of  $f_l(k)$  at  $k = 0$  can correspond to a bound state [13, 14].

Finally, we mention an important result obtained by Bargmann [16]: the number  $n_l$  of bound states of angular momentum  $l$  satisfies the inequality

$$n_l < (2l + 1)^{-1} \int_0^\infty dr \, r |U(r)|. \quad (11.55)$$

Let us illustrate our study of the analytic properties of the Jost functions on a simple example. We consider the case of s-wave scattering by a square well potential

$$U(r) = \begin{cases} -U_0, & r < a \\ 0, & r > a. \end{cases} \quad (U_0 > 0) \quad (11.56)$$

For  $r > a$ , we find from eq. (11.9) that the function  $f(k, r)$  is given by

$$f(k, r) = e^{-ikr}, \quad r > a. \quad (11.57)$$

In the “interior” region  $r < a$  we have

$$f(k, r) = C_1(k) e^{ikr} + C_2(k) e^{-ikr}, \quad r < a \quad (11.58)$$

where  $C_1(k)$  and  $C_2(k)$  are two constants (for fixed  $k$ ) and we have defined the quantity

$$\kappa = \sqrt{k^2 + U_0}. \quad (11.59)$$

In order to determine the “constants”  $C_1$  and  $C_2$  we use the fact that the function  $f(k, r)$  and its first derivative with respect to  $r$  are continuous at  $r = a$ . That is,

$$C_1 e^{ika} + C_2 e^{-ika} = e^{-ika}$$

and

$$ikC_1 e^{ika} - ikC_2 e^{-ika} = -ik e^{-ika} \quad (11.60)$$

so that

$$C_1(k) = \frac{\kappa - k}{2\kappa} e^{-i(\kappa+k)a} \quad (11.61)$$

and

$$C_2(k) = \frac{\kappa + k}{2\kappa} e^{i(\kappa-k)a}.$$

Hence the Jost function  $f(k)$  is given by

$$f(k) = C_1 + C_2 = e^{-ika} \left[ \cos \kappa a + \frac{ik}{\kappa} \sin \kappa a \right]. \quad (11.62)$$

We verify from eq. (11.62) that  $\mathcal{J}(k)$  is an entire function of  $k$  [cf. the discussion following eq. (11.24)]. The zeros of  $\mathcal{J}(k)$  appearing on the negative imaginary axis at the locations  $k = -ik_n$  ( $k_n > 0$ ) are found by solving the equation

$$\xi \cot \xi = -\eta \quad (11.63)$$

where

$$\xi = \kappa_n a, \quad \eta = k_n a \quad (11.64)$$

and

$$\kappa_n = \sqrt{U_0 - k_n^2}.$$

The relation (11.63) is precisely the well-known condition which determines the  $l = 0$  bound states of the square well (11.56) having energies  $E_n = -\hbar^2 k_n^2 / 2m$  [see e.g. 17].

## 11.2. The $S$ -matrix

The physical solution  $u_l(k, r)$  of eq. (11.46) has been shown in Chapter 4 to have the asymptotic behaviour

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} A_l(k) \sin[kr - \frac{1}{2}l\pi + \delta_l(k)] \quad (11.65)$$

where  $\delta_l(k)$  is the phase shift for an angular momentum  $l$ . We have also decomposed the right-hand side of eq. (11.65) into radially ingoing and outgoing waves as [see eq. (4.48)]

$$u_l(k, r) \xrightarrow{r \rightarrow \infty} \tilde{A}_l(k) [ -(-)^l e^{-ikr} + S_l(k) e^{ikr} ] \quad (11.66)$$

where  $\tilde{A}_l(k)$  is given by eq. (4.49) and we recall that the  $S$ -matrix elements

$$S_l(k) = \exp\{2i\delta_l(k)\} \quad (11.67)$$

are the coefficients of the outgoing waves and are determined by the collision process. From the definition (11.67) we first note that

$$|S_l| = 1 \quad (11.68)$$

so that the  $S$ -matrix elements  $S_l$  belong to a *unitary* matrix [18].

We now specialize again to s-wave scattering, dropping consistently the subscript  $l = 0$  [i.e.  $S(k) \equiv S_0(k)$ ,  $\delta(k) \equiv \delta_0(k)$ ,  $A(k) \equiv A_0(k)$ , etc]. Let us return to the solution  $\phi(k, r)$ . Since the two regular solutions  $\phi(k, r)$  and  $u(k, r)$  are clearly proportional we may set

$$u(k, r) = \alpha(k) \phi(k, r). \quad (11.69)$$

Then, using eq. (11.66) with  $l = 0$ , we find that

$$\phi(k, r) \xrightarrow{r \rightarrow \infty} B(k) [S(k) e^{ikr} - e^{-ikr}], \quad (11.70)$$

where  $B(k) = \alpha^{-1}(k) \tilde{A}(k)$ .



Let us consider eq. (11.31) in the limit  $r \rightarrow \infty$ . Using the boundary conditions (11.9), we have

$$\phi(k, r) \xrightarrow{r \rightarrow \infty} \frac{1}{2ik} [\not f(k) e^{ikr} - \not f(-k) e^{-ikr}]. \quad (11.71)$$

Hence, by comparison with eq. (11.70) we may express the  $S$ -matrix element  $S(k)$  in terms of the Jost functions as

$$S(k) = \frac{\not f(k)}{\not f(-k)}. \quad (11.72)$$

Since  $\not f(k) \rightarrow 1$  as  $|k| \rightarrow \infty$  and  $\text{Im } k \leq 0$ , we deduce immediately that  $S(k) \rightarrow 1$  for  $k \rightarrow \pm \infty$ . Furthermore, for real  $k$  we see from eq. (11.33) that

$$S(-k) = S^*(k) = \frac{1}{\overline{S(k)}}. \quad (11.73)$$

More generally, for complex  $k$  we also note from eqs. (11.33) and (11.72) that

$$S^*(k^*) = \frac{1}{\overline{S(k)}}. \quad (11.74)$$

We recall in this connection that eq. (11.33) is a particular case of eq. (11.25) which implies that the condition (11.21) holds. If this condition is not realized we are in general not allowed to continue  $S(k)$  off the real  $k$ -axis and to relate  $S(k)$  from positive to negative values of  $k$ .

If we set

$$\not f(\pm k) = |\not f(\pm k)| \exp\{i\varphi(\pm k)\} \quad (11.75)$$

and use again eq. (11.33) we obtain, for real  $k$

$$\not f^*(k) = |\not f(k)| \exp\{-i\varphi(k)\} = \not f(-k) \quad (11.76)$$

so that

$$|\not f(k)| = |\not f(-k)| \quad (11.77)$$

and

$$\varphi(k) = -\varphi(-k). \quad (11.78)$$

Next, from eqs. (11.67) and (11.72) we have  $\varphi(k) \equiv \delta(k)$  [modulo  $\pi$ ], so that the Jost functions  $\not f(\pm k)$  may be written as

$$\not f(\pm k) = |\not f(\pm k)| \exp\{i\delta(\pm k)\} \quad (11.79)$$

with

$$\delta(k) = -\delta(-k). \quad (11.80)$$

It is interesting to evaluate the quantity  $\alpha(k)$  appearing in eq. (11.69). We find that

$$\alpha(k) = kA(k)/|\not f(k)| \quad (11.81)$$

so that the ratio of the radial wave function to the corresponding unperturbed solution (no interaction), computed at  $r = 0$ , is simply

$$\mathcal{F} = \left[ \frac{u(k, r)}{A(k) \sin kr} \right]_{r=0} = \frac{\alpha(k) \phi'(k, 0)}{k A(k)} = \frac{1}{|\mathcal{J}(k)|}. \quad (11.82)$$

The quantity  $|\mathcal{F}|^2$  which measures the probability of finding the particle at  $r = 0$  relative to that when there is no interaction, is called the *enhancement factor* [19]. It is seen from eq. (11.82) to be the inverse of the modulus squared of the Jost function.

We now study the *analytic properties* of the  $S$ -matrix element  $S(k)$ . The basis of this analysis is provided by the properties of the Jost functions discussed above. However, since  $S(k) = \mathcal{J}(k)/\mathcal{J}(-k)$ , the discussion of the analytic properties of  $S(k)$  is clearly more difficult.

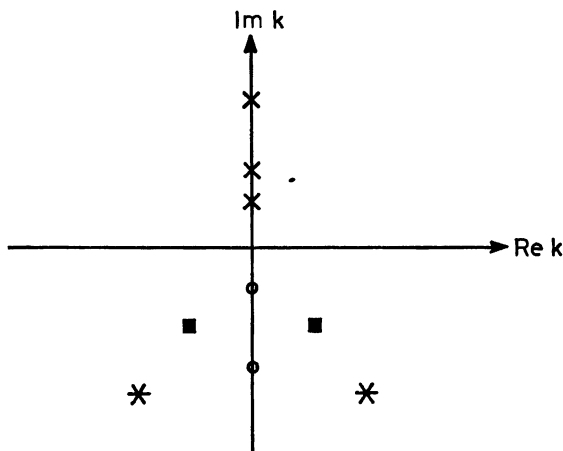


Fig. 11.3. The poles of  $S(k)$  for a potential with a strict finite range.  $\times$ : Poles corresponding to bound states.  $\blacksquare$ ,  $*$ : Poles appearing by pairs in the lower half-plane.  $\circ$ : Poles on the negative imaginary axis.

We begin by considering the simple case for which the potential vanishes identically beyond a certain distance. In this case the functions  $\mathcal{J}(\pm k)$  are both regular in the  $k$ -plane so that the only singularities of  $S(k)$  are *poles* which arise from the zeros [20] of  $\mathcal{J}(-k)$ . The poles in the upper half-plane are thus located on the positive imaginary axis and correspond to bound states (see Fig. 11.3). In the lower half-plane the poles lie either on the negative imaginary axis or by symmetrical pairs about it. There can be no pole of  $S(k)$  for  $k$  real  $\neq 0$ . It is interesting to note that the poles of  $S(k)$  also show up as zeros of  $S(-k)$  because in this simple case the analytic continuation from positive to negative  $k$  values is allowed.

If the potential only satisfies the condition (11.21), both  $f(k)$  and  $f(-k)$  are regular within the strip

$$-\frac{1}{2}\mu < \text{Im } k < \frac{1}{2}\mu. \quad (11.83)$$

Within this "analyticity strip", one can prove [20] that  $f(k)$  does not vanish at the same points as  $f(-k)$ , so that the poles of  $S(k)$  correspond to the zeros of  $f(-k)$ . Outside the analyticity strip, however, other singularities (poles, branch cuts) may appear. Also, if for a value  $k_0 = -i|k_0|$  such that  $|k_0| > \frac{1}{2}\mu$  the Jost function  $f(-k_0)$  is infinite while  $f(k_0)$  is finite,  $S(k_0)$  will vanish but this zero will not correspond to a bound state pole at  $i|k_0|$ . Indeed, such a redundant zero disappears if we cut off the potential at an arbitrary large distance, thereby eliminating the singularities of the Jost functions [21].

We have already seen that the poles  $k_n = i|k_n|$  of  $S(k)$  lying on the positive imaginary axis within the analyticity strip correspond to bound states of energy  $E_n = -\hbar^2|k_n|^2/2m$ . We now show that the residues of these poles are directly related to the bound state wave functions. These are given by

$$u_n(r) = \alpha_n \phi(i|k_n|, r) \quad (11.84)$$

or

$$u_n(r) = \beta_n f(-i|k_n|, r) \quad (11.85)$$

so that

$$u_n(r) \xrightarrow{r \rightarrow \infty} \beta_n \exp\{-|k_n|r\}. \quad (11.86)$$

From eq. (11.36) we also have

$$f(-i|k_n|, r) = C_n \phi(-i|k_n|, r) = C_n \phi(i|k_n|, r). \quad (11.87)$$

Thus  $\alpha_n = \beta_n C_n$ . Moreover, from the requirement that the bound state wave functions  $u_n(r)$  be normalized to one we deduce that

$$\alpha_n^2 = \frac{2|k_n|C_n}{\frac{d}{d|k_n|}f(-i|k_n|)} = - \frac{4|k_n|^2}{f(i|k_n|) \left[ \frac{d}{d|k_n|}f(-i|k_n|) \right]} \quad (11.88)$$

where we have used eqs. (11.37) and (11.45). Hence

$$\beta_n^2 = \frac{\alpha_n^2}{C_n^2} = \frac{i f(i|k_n|)}{\left[ \frac{d}{dk} f(-k) \right]_{k=i|k_n|}}. \quad (11.89)$$

Finally, by using eq. (11.72) together with the Cauchy theorem we deduce that

$$\text{Res } S(k)|_{k=i|k_n|} = \frac{1}{2\pi i} \oint_C S(k) dk = -i\beta_n^2 \quad (11.90)$$

where the contour  $C$  is a small circle described by the complex variable  $k$  in the conventional positive sense around the pole at  $k = i|k_n|$ . We see from eq. (11.90) that the residue of  $S(k)$  at the bound state pole  $k = i|k_n|$  is indeed related to the corresponding wave function.

We now consider briefly the case of higher angular momenta. First of all, we note from eqs. (11.48) and (11.50) that

$$\phi_l(k, r) \xrightarrow{r \rightarrow \infty} \frac{1}{2ik} [\tilde{f}_l(k) e^{ikr} - \tilde{f}_l(-k) e^{-ikr}], \quad (11.91)$$

an obvious generalization of eq. (11.71). Then, from eq. (11.66) and the fact that the two regular solutions  $u_l(k, r)$  and  $\phi_l(k, r)$  are proportional, we have

$$S_l(k) = e^{i\pi l} \tilde{f}_l(k)/\tilde{f}_l(-k) \quad (11.92)$$

or using eq. (11.54),

$$S_l(k) = \frac{f_l(k)}{f_l(-k)}. \quad (11.93)$$

Most of the results found above for the case  $l = 0$  are unchanged. For example  $S_l(k) \rightarrow 1$  for  $k \rightarrow \pm \infty$ . Moreover, for real  $k$ , we may use eq. (11.51) – which implies that the condition (11.21) holds – to deduce that

$$S_l(-k) = S_l^*(k) = \frac{1}{S_l(k)}. \quad (11.94)$$

We also have

$$f_l(\pm k) = |f_l(\pm k)| \exp\{i\delta_l(\pm k)\} \quad (11.95)$$

with

$$\delta_l(k) = -\delta_l(-k). \quad (11.96)$$

For complex  $k$ , eq. (11.51) also yields

$$S_l^*(k^*) = \frac{1}{S_l(k)}. \quad (11.97)$$

Moreover, for potentials satisfying the condition (11.21), the  $S$ -matrix  $S_l(k)$  is analytic in the strip (11.83), except for poles corresponding to the zeros of  $f_l(-k)$ .

Instead of discussing the analytic properties of the  $S$ -matrix as a function of  $k$ , it is also instructive to visualize the  $S$ -matrix as a function of the energy  $E = \hbar^2 k^2/2m$ . We shall write here somewhat loosely  $S_l(k) = S_l(E)$ . As in the discussion following eq. (5.116), it will prove convenient to consider the energy plane as made up of two superposed planes (Riemann sheets), which correspond to two choices of  $\text{Im } k$ . For  $\text{Im } k > 0$  we recall that we are on the *physical sheet* while  $\text{Im } k < 0$  corresponds to the *unphysical sheet*. The two sheets having the common boundary  $\text{Im } k = 0$ , we shall consider the complex  $E$ -plane as cut along the real axis from 0 to  $+\infty$  (see Fig. 5.4). If the potential satisfies the condition (11.21), the  $S$ -matrix may be continued to complex energies inside the parabola

$$(\text{Im } E)^2 - (\hbar^2 \mu^2/2m) \text{Re } E - \hbar^4 \mu^4/16m^2 = 0 \quad (11.98)$$

which corresponds to the analyticity strip  $|\text{Im } k| < \frac{1}{2}\mu$  in the  $k$ -plane. Within the region defined by (11.98) on the physical sheet the  $S$ -matrix has only simple poles at the bound state energies  $E_n$ .

Consider now a pole of the  $S$  matrix which lies within the analyticity region of the  $k$ -plane at  $k = k_1 - ik_2$  ( $k_1 > k_2 > 0$ ) close to the real axis. Then  $S_l(k)$  has also a pole at  $k = -k_1 - ik_2$  and a zero at  $k = k_1 + ik_2$ . We may thus write

$$S_l(k) = \frac{k - k_1 - ik_2}{k - k_1 + ik_2} \tilde{S}_l(k) \quad (11.99)$$

where  $\tilde{S}_l(k)$  is a slowly varying function in the vicinity of  $k = k_1 - ik_2$ . Remembering that  $S_l(k) = \exp(2i\delta_l)$  and setting

$$\delta_l(k) = \xi_l(k) + \delta_l^r(k) \quad (11.100)$$

[see eq. (4.216)], we find that

$$\exp\{2i\xi_l(k)\} = \tilde{S}_l(k) \quad (11.101)$$

and

$$\delta_l^r(k) = \tan^{-1} \frac{k_2}{k_1 - k}. \quad (11.102)$$

Thus  $\delta_l^r(k)$  sharply increases by an amount  $\pi$  in an interval of approximate width  $k_2$  about  $k_1$ , and goes through  $\frac{1}{2}\pi$  (modulo  $\pi$ ) at  $k = k_1$ . Such a behaviour is characteristic of a resonance as we have seen in Chapter 4.

We now translate these results into the *energy plane*. Since  $\text{Im } k < 0$  we are on the unphysical sheet. Moreover, we remain within the parabola given by eq. (11.98). Defining

$$E_r = \frac{\hbar^2}{2m}(k_1^2 - k_2^2), \quad (11.103)$$

and

$$\Gamma = \frac{2\hbar^2}{m}k_1k_2 \quad (11.104)$$

with  $k_1 > k_2 > 0$ , we may now write

$$S_l(E) = \frac{E - E_r - \frac{1}{2}i\Gamma}{E - E_r + \frac{1}{2}i\Gamma} \tilde{S}_l(E). \quad (11.105)$$

If we set

$$\delta_l(E) = \xi_l(E) + \delta_l^r(E) \quad (11.106)$$

then

$$\exp\{2i\xi_l(E)\} = \tilde{S}_l(E) \quad (11.107)$$

and

$$\delta_l^r(E) = \tan^{-1} \frac{\frac{1}{2}\Gamma}{E_r - E} \quad (11.108)$$

so that a pole at  $E = E_r - \frac{1}{2}i\Gamma$  on the unphysical sheet produces a resonance of width  $\Gamma$  and energy  $E_r$ , provided  $\Gamma$  is not too large (i.e. the pole lies close to the real axis). The fact that both bound states and resonances are connected with poles of the  $S$  matrix suggests a strong similarity between these

two concepts. In Chapter 4 we have already seen that resonances can be interpreted as metastable states with a lifetime  $\tau \simeq \hbar/\Gamma$ . The analogy between bound states and resonances has been further developed in modern theories of “elementary” particles, where poles of the relevant  $S$  matrix on the real axis of the energy plane (stable particles) and complex poles (unstable particles) are treated on the same footing [see e.g. 4].

Until now we have only considered potentials which vanish identically beyond  $r = a$  or satisfy the condition (11.21). It may happen that  $U(r)$  does not obey the inequality (11.21) for  $\mu > \mu_0$  but that the region of analyticity of the  $S$  matrix may still be enlarged outside the strip  $|\operatorname{Im} k| < \frac{1}{2}\mu_0$ . For example, in the case of an exponential potential  $U(r) = U_0 \exp(-\alpha r)$  one finds that the Jost function  $f(-k)$  has no singularities in the lower half-plane except for simple poles at  $k = -\frac{1}{2}i\alpha n$  ( $n = 1, 2, \dots$ ). For a Yukawa potential  $U(r) = U_0 \exp(-\alpha r)/r$ , the Jost function  $f(-k)$  has a (logarithmic) branch point at  $k = -\frac{1}{2}i\alpha$ . More generally, for a superposition of Yukawa potentials of the form

$$U(r) = \int_{v_0 > 0}^{\infty} dv \rho(v) e^{-vr}/r \quad (11.109)$$

the Jost function  $f(-k)$  is regular in the complex  $k$ -plane (provided that  $\rho(v)$  decreases fast enough as  $v \rightarrow \infty$ ) except for a cut running from  $k = -\frac{1}{2}iv_0$  to  $-i\infty$ . In the energy plane, this cut runs from  $E = -\hbar^2 v_0^2/8m$  to  $E = -\infty$  and is often called the *left-hand cut*. The *right-hand cut*, which separates the physical and unphysical sheets, runs from  $E = 0$  to  $E = +\infty$ .

To conclude this section, we note that the analytic properties of the partial wave amplitudes

$$a_l = \frac{1}{k} \exp(i\delta_l) \sin \delta_l = \frac{1}{2ik} [\exp(2i\delta_l) - 1] = \frac{1}{2ik} (S_l - 1) \quad (11.110)$$

[see eq. (4.65)] are given by those [22] of the  $S$  matrix  $S_l = \exp(2i\delta_l)$ . For example, in the case of a superposition of Yukawa potentials, the singularities of the quantities  $a_l$  in the energy plane are

- 1) A right-hand cut from  $E = 0$  to  $E = +\infty$ .
- 2) A left-hand cut from  $E = -\hbar^2 v_0^2/8m$  to  $E = -\infty$ .
- 3) Poles on the physical sheet at the bound state energies.
- 4) Poles on the unphysical sheet, among which those lying close to the positive real axis may be interpreted as resonances.

### 11.3. The Levinson theorem

As an application of the analyticity properties studied above, we shall now find the relation between the zero-energy value of the phase shift and the number of bound states. Let us assume that the Jost function  $f(-k)$  has  $n$

zeros in the domain  $D$  enclosed by the contour  $C$  (see Fig. 11.4). This contour consists of a semi-circle of radius  $R$  in the upper half-plane, plus the real axis from  $-R$  to  $+R$ , except the origin which is avoided along a semi-circle of radius  $\varepsilon$ . Then, since  $f(-k)$  is analytic in the upper half- $k$ -plane, where it has simple zeros corresponding to the bound states, we find by using the argument theorem [23] that the quantity

$$n = \frac{1}{2\pi i} \oint_C d \log f(-k) \quad (11.111)$$

yields the number of bound states of zero angular momentum. Because  $f(-k) \rightarrow 1$  as  $|k| \rightarrow \infty$  when  $\text{Im } k \geq 0$ , the large semi-circle does not contribute to the integral (11.111) in the limit  $R \rightarrow \infty$ . To evaluate the contribution from the small semi-circle as  $\varepsilon \rightarrow 0$  we must distinguish two cases. If  $f(0) \neq 0$  there is evidently no contribution. If  $f(0) = 0$ , we know that  $f(k)$  tends to zero as  $k$  [see eq. (11.40)]; the contribution from the small semi-circle is then given by

$$\int d \log k = i\pi. \quad (11.112)$$

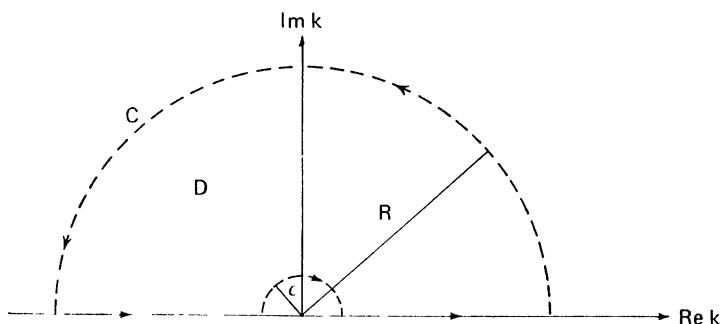


Fig. 11.4. The integration contour of eq. (11.111).

Using eq. (11.79), we now obtain from eq. (11.111)

$$\lim_{\substack{\varepsilon \rightarrow 0^+ \\ R \rightarrow \infty}} \left\{ -\delta(R) + \delta(\varepsilon) - \delta(-\varepsilon) + \delta(-R) + i \log \left| \frac{f(R)}{f(-R)} \frac{f(-\varepsilon)}{f(\varepsilon)} \right| \right\} \\ = \begin{cases} 2\pi(n + \frac{1}{2}), & \text{if } f(0) = 0 \\ 2\pi n, & \text{if } f(0) \neq 0 \end{cases} \quad (11.113)$$

The imaginary part of the left-hand side vanishes because of eq. (11.33). Using eq. (11.80) and the fact that  $\delta(\infty) = 0$ , we then obtain the result

$$\delta(0) = \begin{cases} (n + \frac{1}{2})\pi, & \text{if } f(0) = 0 \\ n\pi, & \text{if } f(0) \neq 0 \end{cases} \quad (11.114)$$

which is the *Levinson theorem*. This proof can easily be extended to the case  $l \geq 1$ . Using the fact that  $f_l(k)$  tends to zero as  $k^2$ , one obtains

$$\delta_l(0) = n_l \pi \quad (11.115)$$

where  $n_l$  denotes the total number of bound states of angular momentum  $l$ , including those at zero binding energy [24].

### 11.4. Complex angular momenta – Regge poles

We have analyzed so far the analytic properties of scattering amplitudes as functions of complex wave numbers and energies. For example, we found that the partial wave scattering amplitudes  $a_l$  are analytic functions of the energy  $E$ , except for possible poles (corresponding to bound states and resonances) and cuts. In this analysis the angular momentum quantum number  $l$  always took its discrete, physically allowed values  $l = 0, 1, 2, \dots$ . The basic idea of Regge [7] was to observe that the radial Schrödinger equation depends in a simple way on the angular momentum  $l$ , so that one could analyze its solutions for continuous and even complex values of  $l$ . This, of course, does not mean that the quantization of the angular momentum has been abandoned. The investigation of Regge provides a new mathematical device to analyze scattering experiments, which also yields a great deal of additional physical insight. Although the method is useful in non-relativistic scattering theory, its main interest lies in high-energy particle physics. We shall only outline here the method for non-relativistic potential scattering. Additional developments may be found in the references [25–29] listed at the end of this chapter. A simple application of the Regge theory to high-energy particle physics will be described in Chapter 18.

Let us consider a superposition of Yukawa potentials [30]

$$U(r) = \int_{v_0 > 0}^{\infty} \rho(v) \frac{e^{-vr}}{r} dv \quad (11.116)$$

and analyze the properties of the  $S$  matrix as a function of the complex variable  $l$ . We first note that the regular solution  $\phi_l(k, r)$ , which we rewrite as  $\phi(l, k, r)$ , is a regular function of  $l$  only in the domain  $\text{Re } l > -\frac{1}{2}$ . Indeed, the boundary condition for the regular solution is given by eq. (11.47), namely

$$\lim_{r \rightarrow 0} r^{-l-1} \phi(l, k, r) = 1 \quad (11.117)$$

while the irregular solution behaves as  $r^{-l}$  at  $r = 0$ . Therefore, when  $\text{Re } l < -\frac{1}{2}$ , the boundary condition (11.117) does not prevent an arbitrary admixture of the irregular solution at  $r = 0$ .

Consider now the irregular solutions  $f(l, \pm k, r) \equiv f_l(\pm k, r)$ . Because the boundary condition (11.48) is independent of  $l$  these functions are *regular* in



the entire complex  $l$ -plane, for fixed values of  $r$  and for fixed  $k$  not lying on the "Yukawa cuts" extending from  $k = \frac{1}{2}iv_0$  to  $+i\infty$  for  $f(l, k, r)$  and from  $k = -\frac{1}{2}iv_0$  to  $-i\infty$  for  $f(l, -k, r)$ .

These analyticity properties of the functions  $\phi(l, k, r)$  and  $f(l, \pm k, r)$  imply that the Jost functions  $\mathcal{f}(l, \pm k) \equiv \mathcal{f}_l(\pm k)$  defined by eq. (11.54) are analytic in the  $l$ -plane provided that  $\text{Re } l > -\frac{1}{2}$  and for any fixed  $k$  not on the "Yukawa cuts". The  $S$ -matrix element being given by

$$S(l, k) = \frac{\mathcal{f}(l, k)}{\mathcal{f}(l, -k)} \quad (11.118)$$

the poles of  $S(l, k)$  in the complex  $l$ -plane – called the *Regge poles* – are due to the zeros of  $\mathcal{f}(l, -k)$ . The equation

$$\mathcal{f}(l, -k) = 0 \quad (11.119)$$

then defines  $l = \alpha(k)$  as an analytic function of  $k$  for  $\text{Re } l > -\frac{1}{2}$  provided its values are finite. The functions  $l = \alpha(k)$  are called *Regge pole trajectories*. We shall also write  $l = \alpha(E)$  to denote Regge pole trajectories generated by varying the energy  $E$ .

Let us now try to locate the Regge poles. We assume that the value of  $l$ , lying in the half-plane  $\text{Re } l > -\frac{1}{2}$ , is such that eq. (11.119) is verified. Setting  $\lambda = l + \frac{1}{2}$  (with  $\text{Re } \lambda > 0$ ), we first obtain from the radial Schrödinger equation, for real energies,

$$\frac{d}{dr} W[\phi^*, \phi] = 2i \text{Im } \lambda^2 r^{-2} |\phi|^2 \quad (11.120)$$

where  $W[\phi^*, \phi]$  is the Wronskian of the functions  $\phi^*$  and  $\phi$ . Integration of eq. (11.120) then yields

$$\lim_{r \rightarrow \infty} W[\phi^*, \phi] = 2i \text{Im } \lambda^2 \int_0^\infty dr r^{-2} |\phi|^2. \quad (11.121)$$

Let us first examine the case of negative energies, so that  $k$  is positive imaginary. Since the value of  $l$  is such that eq. (11.119) is true,  $\phi(l, k, r)$  is exponentially decreasing as  $r \rightarrow \infty$ , and the left-hand side of eq. (11.121) vanishes. Because the integral on the right-hand side does not vanish, we must have  $\text{Im } \lambda^2 = 0$ . Hence, for negative energies and for  $\text{Re } \lambda > 0$  one has  $\text{Im } \lambda = 0$ , so that the *Regge poles for negative energies lie on the real  $l$ -axis* (with  $\text{Re } l > -\frac{1}{2}$ ). Furthermore, a reasoning similar to that leading to eq. (11.45) shows that these poles are simple as functions of  $k$ . Finally, one may prove [27, 28] that these poles move towards the right when the energy increases.

We may also use eq. (11.121) to analyze the case of positive energies. Using eq. (11.91) we find that

$$|\tilde{\mathcal{f}}(l, k)|^2 - |\tilde{\mathcal{f}}(l, -k)|^2 = 8k \text{Re } \lambda \text{Im } \lambda \int_0^\infty dr r^{-2} |\phi|^2 \quad (11.122)$$

where  $\tilde{f}(l, k) \equiv \tilde{f}_l(k)$  is the generalized Jost function defined by eq. (11.49). Because the integral on the right-hand side of eq. (11.122) is manifestly positive, we see that  $\tilde{f}(l, -k)$  vanishes in the domain  $\text{Re } \lambda > 0$  only for  $\text{Im } \lambda > 0$  [31]. Therefore, once the threshold  $E = 0$  for scattering processes is reached, the Regge trajectory leaves the real axis and moves into the *first* quadrant of the complex  $\lambda$ -plane. It never penetrates into the fourth quadrant.

As the energy continues to increase, the Regge trajectories may or may not turn over and go back to the left towards the “forbidden region”  $\text{Re } l < -\frac{1}{2}$ , depending on the nature of the potential. We show on Fig. 11.5 a typical Regge trajectory which does turn over.

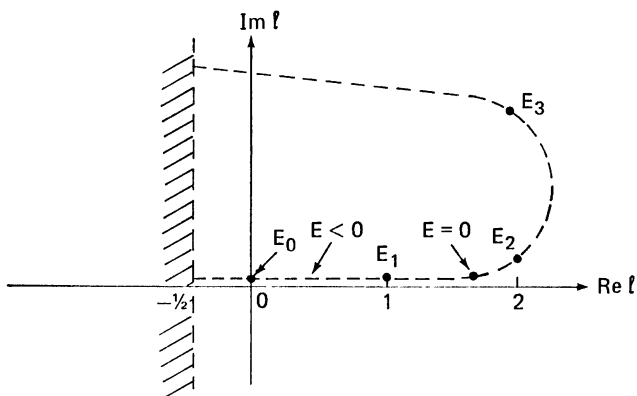


Fig. 11.5. A typical Regge trajectory. The shaded area is the “forbidden region”  $\text{Re } l < -\frac{1}{2}$ . The energies are such that  $E_0 < E_1 < E_2 < E_3$ .

Having studied the Regge trajectories (i.e. the motion of Regge poles with the energy as a parameter) in the complex  $l$ -plane, we now obtain a physical interpretation of Regge poles. Assume first that there is a negative energy  $E_n$  such that the Regge trajectory yields

$$\alpha(E_n) = n \quad (11.123)$$

with  $n$  a non-negative integer. For energies  $E$  close to  $E_n$  we may develop  $\alpha(E)$  as

$$\begin{aligned} \alpha(E) &= \alpha(E_n) + (E - E_n)\alpha'(E_n) + \cdots \\ &\simeq n + (E - E_n)\alpha'(E_n). \end{aligned} \quad (11.124)$$

On the other hand, the partial wave amplitude

$$a(l, E) = \frac{1}{2ik} [S(l, E) - 1] \quad (11.125)$$

having a Regge pole for  $l = \alpha$  may be written in the vicinity of this value of  $l$  as

$$a(l, E) = \frac{R_\alpha(E)}{l - \alpha(E)} + \text{finite terms at } l = \alpha \quad (11.126)$$

where  $R_\alpha(E)$  is the residue of  $a(l, E)$  at  $l = \alpha$ . Using eq. (11.124) in eq. (11.126), we find that

$$a(l, E) \simeq \frac{R_\alpha(E)}{\alpha'(E_n)} \left[ \frac{1}{(l - n)/\alpha'(E_n) - (E - E_n)} \right] \quad (11.127)$$

so that, at the energy  $E = E_n$ , the partial wave amplitude  $a(l = n, E)$  has an *energy pole* which corresponds to a *bound state of angular momentum  $l = n$* .

Therefore, if the Regge trajectory  $\alpha(E)$  goes through a non-negative integer  $n$  for an energy  $E_n < 0$ , this implies a *bound state* of energy  $E_n$  and angular momentum  $l = n$ . For example, the Regge trajectory shown on Fig. 11.5 yields two bound states at  $n = 0$  and  $n = 1$ , the corresponding energies being  $E_0$  and  $E_1$ .

Let us now consider the case  $E > 0$  and assume that there is an energy  $E_m$  such that

$$\operatorname{Re} \alpha(E_m) = m \quad (11.128)$$

with  $m$  a non-negative integer. Since the energy is positive, we know that  $\alpha(E)$  has an imaginary part. We may thus develop  $\alpha(E)$  in the vicinity of  $E = E_m$  as

$$\begin{aligned} \alpha(E) &= \operatorname{Re} \alpha(E) + i \operatorname{Im} \alpha(E) \\ &\simeq m + (E - E_m) \left\{ \frac{d}{dE} [\operatorname{Re} \alpha(E)] \right\}_{E=E_m} + i \operatorname{Im} \alpha(E_m). \end{aligned} \quad (11.129)$$

Assuming that  $\operatorname{Im} \alpha(E_m)$  is small so that no further terms in the development are required, and setting

$$q = \left\{ \frac{d}{dE} [\operatorname{Re} \alpha(E)] \right\}_{E=E_m} \quad (11.130)$$

and

$$\frac{1}{2}\Gamma = \frac{\operatorname{Im} \alpha(E_m)}{q}$$

we find that the partial wave amplitude (11.126) may now be written as

$$a(l, E) \simeq \frac{R_\alpha(E)}{q} \left[ \frac{1}{[(l - m)/q] + E_m - E - \frac{1}{2}i\Gamma} \right]. \quad (11.131)$$

Therefore, the amplitude  $a(l = m, E)$  has an energy dependence characteristic of a *resonance* at  $E = E_m$  with a width  $\Gamma$  and an angular momentum quantum number  $l = m$ . Of course we require  $\Gamma > 0$  or  $q > 0$  (since  $\operatorname{Im} \alpha > 0$ ) and therefore the trajectory must *increase* through the value  $\operatorname{Re} \alpha = m$  when the energy increases. For example, in Fig. 11.5 we have a resonance corresponding to the value  $l = 2$  at the energy  $E = E_2$ , but no resonance at the value  $E = E_3$ .

It is obvious from the preceding considerations that Regge trajectories provide interesting correlations between bound states and (or) resonances

having different angular momenta. These relations arise because the same potential  $U(r)$  describes the scattering in all the angular momentum states, a fact which is not explicitly incorporated in the standard partial wave method. Indeed, the partial wave analysis is unmodified when a different interaction potential acts in each partial wave.

Let us briefly summarize the main results we have obtained so far. By using the solutions of the radial Schrödinger equation for complex  $l$  (subject to  $\text{Re } l > -\frac{1}{2}$ ) we have seen that  $S$ -matrix elements  $S(l, k)$  and therefore the partial wave amplitudes  $a(l, k)$  may be defined for complex  $l$ -values. These partial wave amplitudes are meromorphic functions [32] of  $l$  for  $\text{Re } l > -\frac{1}{2}$ . The poles of  $a(l, k)$  – the Regge poles – occur on the real  $l$ -axis for  $E < 0$  and in the upper half-plane  $\text{Im } l > 0$  for  $E > 0$ . It can be shown that their number is finite for the potentials of the type (11.116) considered here. The corresponding Regge trajectories are generated by the motion of the Regge poles as the energy is varied. If the real part of a Regge trajectory passes through a non-negative integer  $n$  at an energy  $E_n$ , it gives rise to a bound state (if  $E_n < 0$ ) or a resonance (if  $E_n > 0$ ,  $\text{Im } \alpha(E_n)$  is small and  $\text{Re } \alpha(E_n)$  increases through  $E = E_n$ ) having an angular momentum quantum number  $l = n$ .

Let us now explore the consequences of the analytic properties of  $a(l, E)$  as a function of  $l$  – and in particular those arising from the presence of Regge poles – on the partial wave sum (4.64), namely

$$f(E, \cos \theta) = \sum_{l=0}^{\infty} (2l+1) a(l, E) P_l(\cos \theta). \quad (11.132)$$

To this end, we shall use a mathematical device known as the *Sommerfeld-Watson transform*. It first considers the expression (11.132) as the sum of residues of an analytic function and then uses the Cauchy theorem to transform the sum into a contour integral. A deformation of the integration contour will then permit to exhibit explicitly the contributions from the Regge poles to the total scattering amplitude [33].

To carry out such a program, we first show that the series (11.132) can be expressed by the following integral

$$f(E, \cos \theta) = \frac{1}{2i} \int_C \frac{(2l+1) a(l, E) P_l(-\cos \theta)}{\sin \pi l} dl \quad (11.133)$$

taken along the contour  $C$  in the complex  $l$ -plane, as shown in Fig. 11.6. This formula is known as the Sommerfeld-Watson representation of the scattering amplitude.

In order to prove this statement we first need an extension of the functions involved in (11.133) away from integer values of  $l$ . The Legendre polynomials  $P_\nu(z)$  have a “standard” analytic continuation based on the Legendre differential equation. By letting the quantity  $\nu$  become complex in the Legendre

equation, one finds that the regular solution is the hypergeometric function [see e.g. 34]

$$P_\nu(z) = {}_2F_1(-\nu, \nu + 1; 1; \tfrac{1}{2}(1 - z)) \quad (11.134)$$

which, for fixed  $z$ , is an entire analytic function of  $\nu$ . For fixed  $\nu$ , it is an analytic function of  $z$  everywhere in the finite  $z$ -plane cut from  $z = -\infty$  to  $z = -1$ .

We also want to interpolate the physical partial wave amplitudes  $a(l, k)$  [ $l = 0, 1, 2, \dots$ ] by an analytic function of  $l$  which is regular in the neighbourhood of the real axis. One possible interpolation has already been discussed above: it used the radial Schrödinger equation for complex  $l$ -values (such that  $\text{Re } l > -\frac{1}{2}$ ). This interpolation, similar to the one we just discussed above for the Legendre functions, may be called the *dynamic* interpolation, since it contains the dynamics of the collision process through the radial Schrödinger equation. An infinite number of other interpolations can clearly be found for the partial wave amplitudes or the  $S$ -matrix elements [35]. We shall adopt here the dynamic interpolation and justify it shortly.

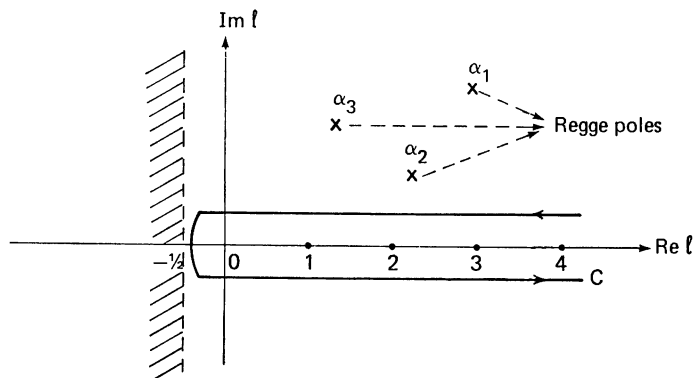


Fig. 11.6. The contour  $C$  used in the evaluation of the integral on the right-hand side of eq. (11.133).

We now return to the integral representation (11.133) of the scattering amplitude. The integrand is analytic for  $\text{Re } l > -\frac{1}{2}$  except for poles which are

i) the Regge poles,

ii) the poles at  $l = n$  ( $n$  non-negative integer) arising from the vanishing of  $\sin \pi l$ . For  $l$  close to  $n$ , we note that

$$\begin{aligned} \sin \pi l &= \sin \pi n + (l - n) \left[ \frac{d}{dl} \sin \pi l \right]_{l=n} + \dots \\ &\simeq (l - n) \pi \cos \pi n = (l - n) \pi (-)^n. \end{aligned} \quad (11.135)$$

Since the contour  $C$  avoids the Regge poles, we may calculate the contour integral (11.133) from the knowledge of the residues of the function  $(\sin \pi l)^{-1}$  at  $l = n$  [36]. Setting

$$g(l) = \frac{\pi(2l + 1)a(l, E)P_l(-\cos \theta)}{\sin \pi l} \quad (11.136)$$

and using eq. (11.135) together with the fact that

$$P_l(-\cos \theta) = (-1)^l P_l(\cos \theta) \text{ at } l = n \quad (11.137)$$

we find that

$$\begin{aligned} \frac{1}{2\pi i} \int_C g(l) dl &= \sum_{n=0}^{\infty} \text{Res } g(l = n) \\ &= \sum_{n=0}^{\infty} \frac{\pi(2n + 1)a(n, E)(-1)^n P_n(\cos \theta)}{\pi(-1)^n} \\ &= \sum_{n=0}^{\infty} (2n + 1)a(n, E)P_n(\cos \theta) \end{aligned} \quad (11.138)$$

where  $\text{Res } g(l = n)$  means the residue of the function  $g(l)$  at  $l = n$ . Hence the series (11.132) can indeed be replaced by the integral (11.133).

In order to exhibit the contribution from the Regge poles to the scattering amplitude, we use again the Cauchy theorem to deform the contour  $C$ . As shown on Fig. 11.7, we now consider the contour  $C'$ , which is made up partly of the previous path  $C$ , but also of portions of a circle in the first and fourth quadrant; the radius of the circle will eventually tend to infinity. The contour  $C'$  also contains the straight line  $\text{Re } l = -\frac{1}{2} + \varepsilon$ , with  $\varepsilon$  a small, positive quantity so that we always stay in the "allowed" domain  $\text{Re } l > -\frac{1}{2}$ . Applying the residue theorem to this new contour we find that

$$\frac{1}{2\pi i} \oint_{C'} g(l) dl = - \sum_i \text{Res } g(l = \alpha_i) \quad (11.139)$$

where the sum runs over all the Regge poles inside the contour  $C'$ , and the minus sign arises from the fact that the contour is followed in the negative sense. We may decompose the integral on the left-hand side as

$$\begin{aligned} \frac{1}{2\pi i} \oint_{C'} g(l) dl &= \frac{1}{2\pi i} \left[ \int_C g(l) dl + \int_{\text{large semi-circle}} g(l) dl \right. \\ &\quad \left. + \int_{-i\infty - 1/2 + \varepsilon}^{i\infty - 1/2 + \varepsilon} g(l) dl \right]. \end{aligned} \quad (11.140)$$

According to eq. (11.138), the first term on the right-hand side is simply the scattering amplitude  $f(E, \cos \theta)$ . The second term may be shown to vanish

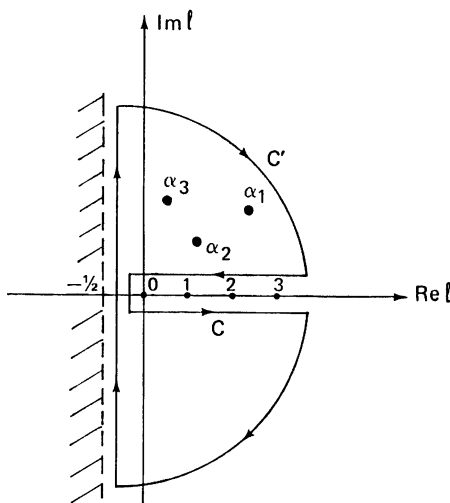


Fig. 11.7. Illustration of the contour  $C'$  of the text.

for potentials of the type (11.116) as the size of the semicircle becomes infinite. Finally, if we define a *background integral* as

$$\text{BI}(E, \cos \theta) = -\frac{1}{2\pi i} \int_{-i\infty - 1/2 + \varepsilon}^{i\infty - 1/2 + \varepsilon} g(l) dl \quad (11.141)$$

and use eqs. (11.139) and (11.140), we find that the scattering amplitude may be expressed as

$$f(E, \cos \theta) = - \sum_i \text{Res } g(l = \alpha_i) + \text{BI}(E, \cos \theta) \quad (11.142)$$

i.e. as a sum over the Regge poles to the right of  $\text{Re } l = -\frac{1}{2}$  plus a background integral. The Regge pole contribution may be displayed in a more explicit way by calculating the residue of  $g(l)$  at  $l = \alpha_i$ . If  $\alpha_i$  is not an integer [37] we may use eqs. (11.126) and (11.136) to write

$$\text{Res } g(l = \alpha_i) = - \frac{\beta_i(E) P_{\alpha_i(E)}(-\cos \theta)}{\sin \pi \alpha_i(E)} \quad (11.143)$$

with

$$\beta_i(E) = -\pi[2\alpha_i(E) + 1]R_{\alpha_i(E)} \quad (11.144)$$

so that eq. (11.142) becomes

$$f(E, \cos \theta) = \sum_i \frac{\beta_i(E) P_{\alpha_i(E)}(-\cos \theta)}{\sin \pi \alpha_i(E)} + \text{BI}(E, \cos \theta). \quad (11.145)$$

This important formula is known as the *Regge-Sommerfeld-Watson* (RSW) *representation of the scattering amplitude*. It allows one to analyze explicitly the contribution to the total scattering amplitude from each Regge pole. We shall see in Chapter 18 how the RSW representation is particularly

useful in describing high-energy collisions of elementary particles. We note that the physical interpretation of Regge poles given above may be recovered by extracting the physical partial wave amplitudes from eq. (11.145) as

$$a_l(E) = \frac{1}{2} \int_{-1}^{+1} dz f(E, z) P_l(z). \quad (11.146)$$

Using the fact [38] that when  $l = m$  is a non-negative integer

$$\int_{-1}^{+1} dz P_m(z) P_\alpha(-z) = \frac{2}{\pi} \frac{\sin \pi \alpha}{(\alpha - m)(m + \alpha + 1)} \quad (11.147)$$

we get from the contribution of the  $n$ th Regge pole term in eq. (11.145)

$$a_{l=m}^{(n)}(E) = \frac{\beta_n(E)}{\pi(m + \alpha_n(E) + 1)} \frac{1}{\alpha_n(E) - m}. \quad (11.148)$$

We first note that in general one Regge pole contributes to all partial waves. Furthermore, the particular contribution (11.148) to the  $l = m$  partial wave will dominate the scattering amplitude if  $\alpha_n$  is close to the integer  $m$ . Expanding  $\alpha_n(E)$  about the energy  $E_m$  at which  $\text{Re } \alpha_n = m$ , we find again, as in the discussion [39] following eq. (11.126) that the amplitude  $a_{l=m}^{(n)}$  exhibits an energy dependence characteristic of a *resonance* at  $E = E_m$  provided  $\text{Im } \alpha_n$  is small and the Regge pole moves towards the right through the value  $\text{Re } \alpha_n = m$ . A similar reasoning yields the properties of the *bound states*: for  $E < 0$  and  $\alpha_n(E_m) = m$  the partial wave amplitude  $a_{l=m}^{(n)}$  has an *energy pole* at  $E = E_m$ .

We now return to the uniqueness of the interpolation procedure used to extend the partial wave amplitude – or the  $S$ -matrix element – away from integer values of  $l$ . We have seen above that, from a mathematical point of view, there are an infinite number of possible interpolations. However, *it can be shown* [see e.g. 40] *that any two interpolations of the partial wave amplitude which at infinity behave well enough to allow the RSW representation, and which have only a finite number of poles in the domain  $\text{Re } l > -\frac{1}{2}$  are identical.* The *dynamic* interpolation, based on the radial Schrödinger equation and which we have used in order to obtain eq. (11.145) is therefore the physically “correct” interpolation.

Before we leave the subject of Regge poles in potential scattering, let us analyze the case where the interaction between the two particles [41] includes exchange forces [42] in addition to the ordinary forces. The (space)-exchange potential operator  $V_e^{\text{p}}$  exchanges the space coordinates of the two interacting particles so that its action on the wave function  $\psi(\mathbf{r})$  describing the relative motion is given by

$$V_e^{\text{p}}\psi(\mathbf{r}) = V_e(\mathbf{r})\psi(-\mathbf{r}) \quad (11.149)$$

where  $V_e(\mathbf{r})$  is a function of  $\mathbf{r}$  which we assume to depend only on  $r = |\mathbf{r}|$ . Let us call  $V_d(\mathbf{r})$  the direct (ordinary) potential – which we also assume to be



central - and introduce the reduced potentials  $U_d = 2m V_d/\hbar^2$  and  $U_e = 2m V_e/\hbar^2$ . We may then write the Schrödinger equation in the C.M. system as

$$[\nabla_r^2 + k^2 - U_d(r)]\psi(r) - U_e(r)\psi(-r) = 0. \quad (11.150)$$

Let us decompose the wave functions  $\psi(r)$  and  $\psi(-r)$  in partial waves as

$$\psi(r) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos \theta) \quad (11.151a)$$

and

$$\psi(-r) = \sum_{l=0}^{\infty} R_l(r) P_l(-\cos \theta) = \sum_{l=0}^{\infty} R_l(r) (-1)^l P_l(\cos \theta) \quad (11.151b)$$

where we have used eq. (11.137). Introducing the functions  $u_l(r) = rR_l(r)$  we obtain from eq. (11.150) the radial Schrödinger equation

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U_d(r) - (-1)^l U_e(r) \right] u_l(r) = 0. \quad (11.152)$$

In order to continue eq. (11.152) into the complex  $l$ -plane, we must handle the factor  $(-1)^l$  in front of  $U_e(r)$ . A first approach is to extend  $(-1)^l$  to complex  $l$  by writing it as  $\exp(i\pi l)$  or  $\exp(-i\pi l)$ . In this case, however, we have an exponentially growing potential in the lower or in the upper half  $l$ -plane, so that the RSW representation does not hold any more.

Another possibility is to start from two decoupled sets of radial Schrödinger equations, one for *even* values of  $l$  with a potential

$$V^+(r) = V_d(r) + V_e(r) \quad (11.153)$$

and one for *odd* values of  $l$  with a potential

$$V^-(r) = V_d(r) - V_e(r). \quad (11.154)$$

These radial equations are (with  $U^+ = 2mV^+/\hbar^2$ ,  $U^- = 2mV^-/\hbar^2$ )

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U^+(r) \right] u_l(r) = 0 \quad (l \text{ even}) \quad (11.155a)$$

and

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U^-(r) \right] u_l(r) = 0 \quad (l \text{ odd}). \quad (11.155b)$$

These two independent problems of analytic continuation may now be solved as for the case of an ordinary potential, except that in eq. (11.155a) only the *even* values of  $l$  are *physical*; similarly, only the *odd* values of  $l$  are *physical* in eq. (11.155b). Therefore, a negative energy pole of the  $S$ -matrix corresponding to eq. (11.155a) and going through an *even* integer value of  $l$  implies a physical bound state, while such a pole going through an *odd* integer value of  $l$  does not correspond to a bound state. Similarly, a physical

resonance is generated by a positive energy pole of the  $S$ -matrix corresponding to eq. (11.155a) and passing near an *even* integral value of  $l$ . The same is true, mutatis mutandis, for eq. (11.155b) and odd values of  $l$ . The two equations (11.155) continued in the complex  $l$ -plane as for the case of an ordinary potential will therefore produce two sets of Regge poles  $\alpha_i^+$  and  $\alpha_i^-$  and Regge poles trajectories  $x_i^+(E)$  and  $\alpha_i^-(E)$ . The superscript  $\pm$ , which makes the distinction between the two kinds of poles is called the *signature*. Hence, for Regge trajectories of even signature (+), only the even  $l$  are physical; for pole trajectories of odd signature (-), the odd values of  $l$  are physical. The case of an ordinary (direct) potential is evidently a special case in which the Regge pole trajectories of even and odd signature coincide.

It is convenient to separate the total scattering amplitude  $f(E, \cos \theta)$  corresponding to the scattering of two particles interacting through direct and exchange forces into its *even* and *odd* parts. That is, the relation

$$f(E, \cos \theta) = \sum_{l=0}^{\infty} (2l+1) a(l, E) P_l(\cos \theta)$$

may be written as

$$\begin{aligned} f(E, \cos \theta) &= \sum_{l=0}^{\infty} (2l+1) a(l, E) \left\{ \frac{1}{2} [P_l(\cos \theta) + P_l(-\cos \theta)] \right. \\ &\quad \left. + \frac{1}{2} [P_l(\cos \theta) - P_l(-\cos \theta)] \right\} \quad (11.156) \\ &= f^+(E, \cos \theta) + f^-(E, \cos \theta) \end{aligned}$$

where

$$f^{\pm}(E, \cos \theta) = \frac{1}{2} \sum_{l=0}^{\infty} (2l+1) a^{\pm}(l, E) \{P_l(\cos \theta) \pm P_l(-\cos \theta)\}. \quad (11.157)$$

Since  $P_l(-\cos \theta) = (-)^l P_l(\cos \theta)$ , the amplitude  $f^+$  only contains a sum over *even*  $l$  values, while the sum corresponding to  $f^-$  only contains *odd* values of  $l$ . Accordingly, the only partial wave amplitudes contributing to  $f^+$  are the  $a^+(l, E)$  obtained by solving the Schrödinger equation with the potential  $V^+$ . Similarly, the only partial wave amplitudes which contribute to  $f^-$  are the  $a^-(l, E)$  obtained from the Schrödinger equation with the potential  $V^-$ . Each of the amplitudes  $f^+$  and  $f^-$  can therefore be treated separately to yield a Regge-Sommerfeld-Watson representation. The final result for the total amplitude is [compare with eq. (11.145)]

$$\begin{aligned} f(E, \cos \theta) &= \sum_i \frac{\beta_i^+(E)}{\sin \pi \alpha_i^+(E)} [P_{\alpha_i^+(E)}(-\cos \theta) + P_{\alpha_i^+(E)}(\cos \theta)] \\ &\quad + \sum_j \frac{\beta_j^-(E)}{\sin \pi \alpha_j^-(E)} [P_{\alpha_j^-(E)}(-\cos \theta) - P_{\alpha_j^-(E)}(\cos \theta)] \quad (11.158) \\ &\quad + \tilde{\text{BI}}(E, \cos \theta) \end{aligned}$$

where the functions  $\beta_i^+(E)$  and  $\beta_j^-(E)$  are given by the analogue of eq. (11.144) [except for an extra factor  $\frac{1}{2}$ ] and the background integral  $\tilde{\text{BI}}$  is now given by

$$\tilde{\text{BI}}(E, \cos \theta) = -\frac{1}{4i} \int_{-i\infty-1/2+\varepsilon}^{+i\infty-1/2+\varepsilon} dl \frac{2l+1}{\sin \pi l} \{a^+(l, E)[P_l(-\cos \theta) + P_l(\cos \theta)] + a^-(l, E)[P_l(-\cos \theta) - P_l(\cos \theta)]\}. \quad (11.159)$$

We note that when one of the Regge trajectories  $\alpha_i^+$  goes through an odd value of  $l$  the quantity  $\sin \pi \alpha_i^+$  vanishes; but since  $P_{\alpha_i^+}(-\cos \theta) + P_{\alpha_i^+}(\cos \theta)$  vanishes there also the contribution of this unphysical pole is perfectly regular, as it should be. The same comment applies to  $\alpha_j^-$  when it passes through an even value of  $l$ .

## 11.5. Dispersion relations [43]

### 11.5.1. Introduction

The name "dispersion relation" has its origin in a well known relation between the real part and the imaginary part of the complex index of refraction introduced in optics. Let us first define this complex index of refraction as

$$n(\omega) = \text{Re } n(\omega) + i \text{Im } n(\omega) \quad (11.160)$$

where  $\text{Re } n(\omega)$  is the index of refraction corresponding to the angular frequency  $\omega$  of the incident light, while  $\text{Im } n(\omega)$  is related to the absorption coefficient  $\alpha(\omega)$  of the medium [44] by

$$\text{Im } n(\omega) = \frac{c}{2\omega} \alpha(\omega). \quad (11.161)$$

Classical electrodynamics then relates  $\text{Re } n(\omega)$  to  $\alpha(\omega)$  as

$$\text{Re } n(\omega) = 1 + \frac{c}{\pi} \text{P} \int_0^\infty \frac{\alpha(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (11.162)$$

where P signifies that the principal value [45] of the integral must be taken at the point  $\omega' = \omega$  where the integrand is singular. Kronig [46] and Kramers [47] showed that the requirement that light does not propagate with a velocity greater than  $c$  precisely yields the relation (11.162). Following Kramers' argument, we formally define the index of refraction for negative angular frequencies by

$$n(-\omega) = n^*(\omega) \quad (11.163)$$

so that  $\text{Re } n(\omega)$  is an even function of  $\omega$ ,  $\text{Im } n(\omega)$  is odd and  $\alpha(\omega)$  is even. We may then write eq. (11.162) as

$$\text{Re } n(\omega) - 1 = \frac{c}{\pi} \text{P} \int_{-\infty}^{+\infty} \frac{\alpha(\omega')}{2\omega'(\omega' - \omega)} d\omega' \quad (11.164)$$

or

$$\operatorname{Re}[n(\omega) - 1] = \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Im}[n(\omega') - 1]}{\omega' - \omega} d\omega'. \quad (11.165)$$

This equation, which relates the real and imaginary part of  $n(\omega)$  is called a *dispersion relation*. It is simply the real part of

$$n(\omega) - 1 = \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{n(\omega') - 1}{\omega' - \omega} d\omega'. \quad (11.166)$$

Using the well known relation [48]

$$\lim_{\varepsilon \rightarrow 0^+} \frac{1}{x - x_0 \mp i\varepsilon} = P\left(\frac{1}{x - x_0}\right) \pm i\pi\delta(x - x_0) \quad (11.167)$$

we also find that

$$n(\omega) - 1 = \frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{n(\omega') - 1}{\omega' - \omega - i\varepsilon} d\omega' \quad (11.168)$$

provided  $n(\omega) - 1$  vanishes faster than  $(\log \omega)^{-1}$  for  $\omega \rightarrow \infty$ , so that the integral exists.

This important relation shows that we may define  $n(\omega)$  as a function of a complex variable  $\omega$ , which is analytic in the upper half-plane  $\operatorname{Im} \omega > 0$ . That is,

$$n(\omega) - 1 = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{n(\omega') - 1}{\omega' - \omega} d\omega'. \quad (11.169)$$

Conversely, if we suppose that the function  $n(\omega)$  may be continued to complex values of  $\omega$ , is regular in the upper half-plane  $\operatorname{Im} \omega > 0$  and such that  $n(\omega) - 1$  vanishes as  $|\omega| \rightarrow \infty$ , then eq. (11.169) immediately follows from the Cauchy theorem. Kramers has shown that the required analytic behaviour of  $n(\omega)$  is equivalent to wave propagation through a medium in such a way that no signals are transmitted with a velocity greater than  $c$ . This *causality* requirement therefore imposes the analyticity of the function  $n(\omega)$  and hence the dispersion relation (11.165).

It is instructive to rewrite the dispersion relation (11.165) in terms of the electromagnetic scattering amplitude. Using the classical Lorentz relation

$$n(\omega) = 1 + \frac{2\pi c^2}{\omega^2} N f(\omega) \quad (11.170)$$

where  $N$  is the number of scattering centers per unit volume in the medium and  $f(\omega)$  is the forward scattering amplitude of light at a frequency  $\omega$ , we obtain

$$\operatorname{Re} f(\omega) = \frac{\omega^2}{\pi} P \int_{-\infty}^{+\infty} \frac{\operatorname{Im} f(\omega')}{\omega'^2(\omega' - \omega)} d\omega' = \frac{2\omega^2}{\pi} P \int_0^\infty \frac{\operatorname{Im} f(\omega')}{\omega'(\omega'^2 - \omega^2)} d\omega' \quad (11.171)$$

where we have used the fact that  $\text{Im } f(-\omega) = -\text{Im } f(\omega)$ . The total scattering cross section  $\sigma(\omega)$  of light is related to the imaginary part of the forward scattering amplitude  $\text{Im } f(\omega)$  by the optical theorem

$$\sigma(\omega) = \frac{4\pi c}{\omega} \text{Im } f(\omega) \quad (11.172)$$

with  $\omega = kc$ . Therefore eq. (11.171) may be written as

$$\text{Re } f(\omega) = \frac{\omega^2}{2\pi^2 c} \text{P} \int_0^\infty \frac{\sigma(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (11.173)$$

so that *the knowledge of the total scattering cross section at all frequencies yields the forward scattering amplitude at any frequency*. It is important to note that this result is only true if  $f(\omega) = 0$  for  $\omega = 0$  since otherwise  $n(\omega) - 1$  would have a pole at  $\omega = 0$ . Moreover, we recall that the function  $n(\omega) - 1$  must vanish as  $|\omega| \rightarrow \infty$ . Thus eq. (11.173) is only valid in certain cases, for example when light is scattered by *bound* electrons. For *free* electrons, which can respond to zero frequency,  $f(0)$  is finite. Moreover, the condition  $n(\omega) - 1 \rightarrow 0$  for  $|\omega| \rightarrow \infty$  is no more satisfied, so that the quantity  $f(\infty)$  is infinite [see eq. (11.170)]. One must then replace eq. (11.171) by

$$\text{Re } f(\omega) - \text{Re } f(0) = \frac{2\omega^2}{\pi} \text{P} \int_0^\infty \frac{\text{Im } f(\omega')}{\omega'(\omega'^2 - \omega^2)} d\omega' \quad (11.174)$$

while eq. (11.173) now reads

$$\text{Re } f(\omega) - \text{Re } f(0) = \frac{\omega^2}{2\pi^2 c} \text{P} \int_0^\infty \frac{\sigma(\omega')}{\omega'^2 - \omega^2} d\omega'. \quad (11.175)$$

These last equations are known as the *Kramers–Kronig dispersion relations*. We note that eq. (11.175) implies that

$$\text{Re } f(\infty) = \text{Re } f(0) - \frac{1}{2\pi^2 c} \int_0^\infty \sigma(\omega') d\omega'. \quad (11.176)$$

It is important to remark that the Kramers–Kronig result (11.175) can be deduced from the relation

$$\text{Re } f(\omega) = \frac{1}{2\pi^2 c} \text{P} \int_0^\infty \frac{\omega'^2 \sigma(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (11.177)$$

if the integral on the right of eq. (11.177) converges. This condition, however, is more stringent than that required by eq. (11.175), so that eq. (11.177) is less general than eq. (11.175). We note in particular that eq. (11.177) yields the result

$$\text{Re } f(0) = \frac{1}{2\pi^2 c} \int_0^\infty \sigma(\omega) d\omega \quad (11.178)$$

which is not valid for the scattering of light by *free* electrons. Indeed, in that case the quantity  $f(0)$  is given by the Thompson amplitude

$$f(0) = -\frac{e^2}{mc^2} \quad (11.179)$$

while the right-hand side of eq. (11.178) is clearly positive. We must then return to the more general Kramers–Kronig result (11.175). The procedure of passing from the stronger (less general) relation (11.177) to the weaker result (11.175) is called a *subtraction*. It is clearly related to the asymptotic behaviour of  $f(\omega)$  as  $|\omega| \rightarrow \infty$ . A detailed study of the subtraction procedure will be given below [see eqs. (11.187)–(11.194)].

Let us now summarize what we have learned from this classical example. Starting with the *principle of microcausality* that no signals propagate at velocities faster than  $c$ , we have obtained dispersion relations which relate the index of refraction to the absorption coefficient or the real part of the forward scattering amplitude to the total cross section. We note that no detailed knowledge of electromagnetic theory is necessary to establish these dispersion relations.

The importance of the work of Kronig and Kramers for quantum mechanical scattering processes was not realized for a long time until Kronig [49] pointed out that microscopic causality should impose limitations on the  $S$ -matrix. This problem was further analyzed by several authors [50–52], and a derivation of the Kramers–Kronig relation from quantum field theory was proposed by Gell-Mann, Goldberger and Thirring [53]. We may remark here that in *elementary particle physics* the interactions cannot in general be characterized by simple potentials, and reliable approximation methods for strong interactions are very difficult to construct. It is then particularly interesting to rely on dispersion relations, since these allow one to deduce observable consequences without making *specific* assumptions about the nature of the interactions and to *relate seemingly different physical quantities* (such as the index of refraction and the absorption coefficient in our classical example). New approximation methods based on dispersion relations may then be devised to deal particularly with strong interactions, the greatest success of dispersion relations in elementary particle processes having been obtained in connection with the study of pion–nucleon scattering [54].

Although the importance of dispersion relations is only evident in the study of elementary particle processes, we shall discuss here dispersion techniques within the framework of non-relativistic potential scattering. This will provide an introduction to the subject in a framework where the basic features of the method can be illustrated simply. Before we discuss the non-relativistic theory, however, we shall review some mathematical techniques which are particularly useful in dispersion theory.

### 11.5.2. Mathematical background

We have already analyzed in connection with the Kramers–Kronig formula some of the simplest aspects of dispersion relations. We now discuss in a more systematic way how dispersion relations may be established once the analytic properties of a function are known.

Let us first consider a function  $f(z)$  which is regular for  $\text{Im } z \geq 0$  and such that  $f(z) \rightarrow 0$  when  $|z| \rightarrow \infty$ . Using the Cauchy theorem we obtain

$$f(z) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{f(x')}{x' - z} dx' \quad (11.180)$$

for any  $z$  in the upper half-plane. If we let the point  $z$  approach the real axis, we have

$$f(x) = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{f(x')}{x' - (x + i\varepsilon)} dx' \quad (11.181)$$

which by means of eq. (11.167) becomes

$$f(x) = \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f(x')}{x' - x} dx'. \quad (11.182)$$

Taking the real and imaginary parts of eq. (11.182) we obtain the dispersion relations

$$\text{Re } f(x) = \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im } f(x')}{x' - x} dx' \quad (11.183)$$

and

$$\text{Im } f(x) = -\frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Re } f(x')}{x' - x} dx'. \quad (11.184)$$

Relations such as (11.180)–(11.182) are also often called “dispersion relations”. We note that  $\text{Re } f(x)$  and  $\text{Im } f(x)$  are related by a Hilbert transformation [55].

If the function  $f(x)$  satisfies a relation such as

$$f(-x) = f^*(x) \quad (11.185)$$

[cf. eq. (11.163) for the case of the complex index of refraction], then eq. (11.183) can be written as

$$\text{Re } f(x) = \frac{2}{\pi} P \int_0^{\infty} \frac{x' \text{Im } f(x')}{x'^2 - x^2} dx'. \quad (11.186)$$

The last dispersion relation is particularly useful when  $f(x)$  takes on its “physical” values for positive values of  $x$  only.

We have already encountered in our classical example the case where the function  $f(z)$  does not tend to zero for  $|z| \rightarrow \infty$ . If  $f(z)$  tends to a constant  $f(\infty)$  when  $|z| \rightarrow \infty$ , then we may apply the Cauchy theorem to the function  $f(z) - f(\infty)$  and obtain the “subtracted” form of eq. (11.182), namely

$$f(x) - f(\infty) = \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f(x')}{x' - x} dx' \quad (11.187)$$

where we have used the fact that  $P \int_{-\infty}^{+\infty} (x' - x)^{-1} dx' = 0$ . If we operate the subtraction at  $x = x_0$ , then we find that

$$f(x) - f(x_0) = (x - x_0) \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f(x')}{(x' - x)(x' - x_0)} dx' \quad (11.188)$$

and therefore

$$\operatorname{Re} f(x) - \operatorname{Re} f(x_0) = (x - x_0) \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Im} f(x')}{(x' - x)(x' - x_0)} dx'. \quad (11.189)$$

The subtraction procedure can easily be generalized to the case where the asymptotic behaviour of  $f(z)$  is given by

$$f(z) \rightarrow \sum_{|z| \rightarrow \infty}^n a_j z^j \quad (11.190)$$

so that  $f(z)$  tends to a polynomial of degree  $n$  when  $|z| \rightarrow \infty$ . One then applies the Cauchy theorem to the function  $f(z)/(z' - z_0)^{n+1}$  ( $\operatorname{Im} z_0 > 0$ ) and after taking the limit  $\operatorname{Im} z_0 \rightarrow 0$  one obtains

$$\begin{aligned} f(x) - \sum_{j=0}^n \frac{(x - x_0)^j}{j!} \left( \frac{d^j f}{dx^j} \right)_{x=x_0} \\ = (x - x_0)^{n+1} \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f(x')}{(x' - x)(x' - x_0)^{n+1}} dx' \end{aligned} \quad (11.191)$$

so that  $(n + 1)$  subtractions are necessary in this case.

Next, let us consider the case where the function  $f(z)$  has a finite number  $P$  of poles in the upper half-plane at the points  $z = z_i$ . Calling the corresponding residues  $\Gamma_i$  and assuming that  $f(z) \rightarrow 0$  as  $|z| \rightarrow \infty$ , we now have

$$f(z) = \sum_{i=1}^P \frac{\Gamma_i}{z - z_i} + \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{f(x')}{x' - z} dx'. \quad (11.192)$$

When  $z$  approaches the real axis we use again eq. (11.167) to find that

$$f(x) = \sum_{i=1}^P \frac{2\Gamma_i}{x - z_i} + \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f(x')}{x' - x} dx'. \quad (11.193)$$

If the asymptotic behaviour of  $f(z)$  is given by eq. (11.190) and  $f(z)$  has still  $P$  poles in the upper half-plane, eq. (11.193) is replaced by

$$\begin{aligned} f(x) - \sum_{j=0}^n \frac{(x - x_0)^j}{j!} \left( \frac{d^j f}{dx^j} \right)_{x=x_0} &= \sum_{i=1}^P \frac{2(x - x_0)^{n+1} \Gamma_i}{(x - z_i)(x_0 - z_i)^{n+1}} \\ &+ (x - x_0)^{n+1} \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f(x')}{(x' - x)(x' - x_0)^{n+1}} dx'. \end{aligned} \quad (11.194)$$

We now want to consider the case where the function  $f(z)$  has singularities on the real axis. Isolated poles can be treated by the same method as the



complex poles considered above, but the case of *branch points* is more involved. Suppose for example that  $f(z)$  has a branch point at  $x = a$ , as shown on Fig. 11.8, but that it is otherwise regular in the complex  $z$ -plane. Therefore,  $f(z)$  is analytic in the  $z$ -plane cut (for example) along the real axis from  $x = a$  to  $x = +\infty$ . Applying the Cauchy theorem to the contour  $C$  shown on Fig. 11.8, we find that

$$f(z) = \frac{1}{\pi} \int_a^\infty \frac{\rho(x')}{x' - z} dx' \quad (11.195)$$

where the quantity

$$\rho(x') = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{2i} [f(x' + i\varepsilon) - f(x' - i\varepsilon)] \quad (11.196)$$

is the discontinuity along the branch cut. In particular, if  $f(x)$  is real for  $x \leq a$ , then we may use the Schwarz reflection principle [9] to deduce that

$$\rho(x') = \text{Im } f(x') \quad (11.197)$$

and therefore

$$f(z) = \frac{1}{\pi} \int_a^\infty \frac{\text{Im } f(x')}{x' - z} dx'. \quad (11.198)$$

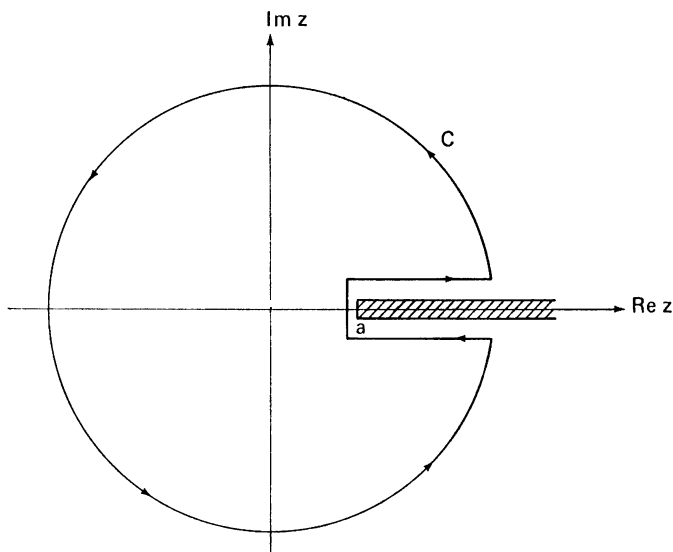


Fig. 11.8. Illustration of the branch point at  $x = a$  and of the contour  $C$ .

If we let  $z$  approach the real axis, but *not on the cut*, we find the dispersion relation

$$f(x) = \text{Re } f(x) = \frac{1}{\pi} \int_a^\infty \frac{\text{Im } f(x')}{x' - x} dx'. \quad (11.199)$$

Complex poles and subtractions can be handled here as before.

### 11.5.3. Dispersion relations in non-relativistic potential scattering

Although there is no limiting velocity in non-relativistic physics, it is nevertheless possible to derive dispersion relations in this case. These were first obtained by Khuri [56] and further developed by several authors [57–59].

Let us start from the integral representation (5.40) of the scattering amplitude and use the compact solution (5.50) in terms of the complete Green's function. We assume that the potential is spherically symmetric. If we denote by  $\Delta = \mathbf{k}_i - \mathbf{k}_f$  the wave vector transfer such that

$$\Delta = |\mathbf{k}_i - \mathbf{k}_f| = 2k \sin \frac{1}{2}\theta \quad (11.200)$$

we may write

$$f(k, \Delta) = -\frac{1}{4\pi} \left[ \int \exp(i\Delta \cdot \mathbf{r}) U(\mathbf{r}) d\mathbf{r} + \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}) U(\mathbf{r}) G^{(+)}(\mathbf{r}, \mathbf{r}', k) U(\mathbf{r}') \exp(i\mathbf{k}_i \cdot \mathbf{r}') d\mathbf{r} d\mathbf{r}' \right], \quad (11.201)$$

where we have displayed explicitly the  $k$ -dependence of the Green's function  $G^{(+)}$ .

We note that the first term on the right-hand side of eq. (11.201) is simply the first Born approximation  $f_{B1}(\Delta)$  to the scattering amplitude. The total Green's function  $G^{(+)}(\mathbf{r}, \mathbf{r}', k)$  has been defined in Section 5.4. It is such that

$$[\nabla_{\mathbf{r}}^2 + k^2 - U(\mathbf{r})] G^{(+)}(\mathbf{r}, \mathbf{r}', k) = \delta(\mathbf{r} - \mathbf{r}') \quad (11.202)$$

and satisfies the integral equation

$$G^{(+)}(\mathbf{r}, \mathbf{r}', k) = G_0^{(+)}(\mathbf{r}, \mathbf{r}', k) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}'', k) U(\mathbf{r}'') G^{(+)}(\mathbf{r}'', \mathbf{r}', k) d\mathbf{r}'' \quad (11.203)$$

with

$$G_0^{(+)}(\mathbf{r}, \mathbf{r}', k) = -\frac{1}{4\pi} \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|}. \quad (11.204)$$

It is important to remark that  $f(k, \Delta)$  is the *physical* amplitude for  $k \geq \frac{1}{2}\Delta$ , as we easily see from eq. (11.200). The physical scattering values of  $k$  are indeed real and positive, with

$$0 \leq \Delta \leq 2k. \quad (11.205)$$

For  $k < \frac{1}{2}\Delta$  we are in the “unphysical region”.

We now want to establish a *dispersion relation* for the scattering amplitude  $f(k, \Delta)$ . We shall only discuss [60] in some detail the case of forward scattering, for which the scattering amplitude  $f(k) \equiv f(k, 0)$  is only a function of the wave number  $k$ . We may then write

$$\tilde{f}(k) = \int \tilde{F}(\mathbf{r}, \mathbf{r}', k) d\mathbf{r} d\mathbf{r}' \quad (11.206)$$

where

$$\tilde{f}(k) = f(k) - f_{B1} \quad (11.207)$$

and  $f_{B1} = -(4\pi)^{-1} \int U(r) dr$  while

$$\tilde{F}(r, r', k) = -\frac{1}{4\pi} \exp(-ik \cdot r) U(r) G^{(+)}(r, r', k) U(r') \exp(ik \cdot r') \quad (11.208)$$

with  $k = k_i = k_f$ .

Starting from the physical scattering amplitude  $f(k)$ , which is defined above for positive real wave numbers  $k$ , we now want to extend the function  $f(k)$  to complex values of  $k$ . To this end we remark that except for possible poles,  $\tilde{F}(r, r', k)$  can be continued into the upper half  $\zeta$  plane,  $\zeta = k + i\varepsilon$ , as an analytic function. Indeed, the total Green's function  $G^{(+)}(r, r', \zeta)$  is analytic [see e.g. 61] in  $\zeta^2$  for almost every  $r, r'$ , except on the spectrum of the Hamiltonian  $H$  where it has discrete *poles* at the values of  $\zeta^2$  corresponding to the bound states, and a *cut* (arising from the scattering states) which runs from 0 to  $+\infty$ . Thus, in the upper-half  $\zeta$ -plane, the only singularities arise from bound states and are located on the imaginary  $\zeta$  axis. Furthermore, if the potential  $U(r)$  is such that

$$\int_0^\infty r |U(r)| dr < \infty$$

then the number  $N$  of such bound states (located at  $\zeta_i = i\kappa_i$ ,  $i = 1, 2, \dots, N$ ) is *finite*.

Let us decompose the Green's function  $G^{(+)}$  as

$$G^{(+)}(r, r', \zeta) = G_B(r, r', \zeta) + G_C^{(+)}(r, r', \zeta) \quad (11.209)$$

where

$$G_B(r, r', \zeta) = \sum_{i=1}^N \frac{\varphi_i(r) \varphi_i^*(r')}{\zeta^2 + \kappa_i^2} \quad (11.210)$$

is the contribution to  $G^{(+)}$  arising from bound states and

$$G_C^{(+)}(r, r', \zeta) = \int d\mathbf{k} \frac{\psi_{\mathbf{k}}^{(+)}(r) \psi_{\mathbf{k}}^{(+)*}(r')}{\zeta^2 - \kappa^2} \quad (11.211)$$

is the continuum contribution to  $G^{(+)}$ . The bound state wave functions  $\varphi_i$  may be chosen to be real, and we have adopted the continuum wave functions  $\psi_{\mathbf{k}}^{(+)}$ , although any complete set – for example the functions  $\psi_{\mathbf{k}}^{(-)}$  – is equally suitable. In addition, since [62]

$$\psi_{-\mathbf{k}}^{(\mp)} = \psi_{\mathbf{k}}^{(\pm)*} \quad (11.212)$$

we note that

$$G^{(+)}(r, r', k) = G^{(+)*}(r', r, -k) \quad (11.213)$$

which implies the symmetry property

$$f(k) = f^*(-k). \quad (11.214)$$

Having isolated  $G_B$  from  $G^{(+)}$ , we have located the only part having singularities for  $\text{Im } \zeta > 0$ . Therefore, if we choose an integration contour  $C$  which consists of that part of the real axis and a large semi-circle, such that

$|\zeta| < A$  and containing all the poles (see Fig. 11.9), we may use the Cauchy theorem to write

$$\frac{1}{2\pi i} \oint_C \frac{\zeta' \tilde{F}(\mathbf{r}, \mathbf{r}', \zeta')}{\zeta'^2 - \zeta^2} d\zeta' = \frac{1}{2} \tilde{F}(\mathbf{r}, \mathbf{r}', \zeta) + \sum_{i=1}^N \frac{\zeta_i \Gamma_i(\mathbf{r}, \mathbf{r}')}{\zeta_i^2 - \zeta^2} \quad (11.215)$$

where  $\Gamma_i(\mathbf{r}, \mathbf{r}')$  is the residue of  $\tilde{F}(\mathbf{r}, \mathbf{r}', \zeta)$  at  $\zeta = \zeta_i$ . We have also used the fact that

$$\frac{\zeta'}{\zeta'^2 - \zeta^2} = \frac{1}{2} \left[ \frac{1}{\zeta' - \zeta} + \frac{1}{\zeta' + \zeta} \right] \quad (11.216)$$

which implies that only the first term on the right contributes to the integral. Using eq. (11.210), we obtain explicitly

$$\Gamma_i(\mathbf{r}, \mathbf{r}') = \frac{1}{2\zeta_i} A_i(\mathbf{r}, \mathbf{r}') \quad (11.217)$$

with

$$A_i(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \lim_{\zeta \rightarrow \zeta_i} [\exp\{i\zeta \mathbf{k}_i \cdot (\mathbf{r}' - \mathbf{r})\} U(\mathbf{r}) U(\mathbf{r}') \phi_i(\mathbf{r}) \phi_i^*(\mathbf{r}')]. \quad (11.218)$$

We may then rewrite eq. (11.215) as

$$\tilde{F}(\mathbf{r}, \mathbf{r}', \zeta) = \sum_{i=1}^N \frac{A_i(\mathbf{r}, \mathbf{r}')}{\zeta^2 - \zeta_i^2} + \frac{1}{\pi i} \oint_C \frac{\zeta' \tilde{F}(\mathbf{r}, \mathbf{r}', \zeta')}{\zeta'^2 - \zeta^2} d\zeta' \quad (11.219)$$

which explicitly displays the analyticity properties of  $\tilde{F}(\mathbf{r}, \mathbf{r}', \zeta)$ .

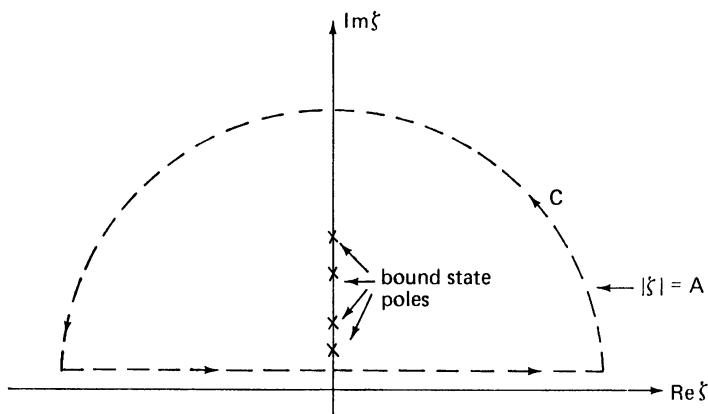


Fig. 11.9. Illustration of the integration contour  $C$  of the text.

We now return to eq. (11.206) which we rewrite in terms of the complex variable  $\zeta$  as

$$\tilde{f}(\zeta) = \int \tilde{F}(\mathbf{r}, \mathbf{r}', \zeta) d\mathbf{r} d\mathbf{r}' \quad (11.220)$$

so that

$$\tilde{f}(k) = \lim_{\varepsilon \rightarrow 0^+} \tilde{f}(\zeta = k + i\varepsilon). \quad (11.221)$$

Hence

$$\tilde{f}(k) = \sum_{i=1}^N \frac{R_i}{\zeta^2 - \zeta_i^2} + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{\pi i} \int d\mathbf{r} d\mathbf{r}' \oint_C \frac{\zeta' \tilde{F}(\mathbf{r}, \mathbf{r}', \zeta')}{\zeta'^2 - \zeta^2} d\zeta' \quad (11.222)$$

where

$$R_i = \int d\mathbf{r} d\mathbf{r}' A_i(\mathbf{r}, \mathbf{r}'). \quad (11.223)$$

From the asymptotic behaviour  $\varphi_i(r) \sim \exp(-\kappa_i r)$  it is easy to see that  $R_i$  is finite at  $\zeta_i = i\kappa_i$ . Furthermore  $R_i$  is real.

In order to obtain a dispersion relation for  $\tilde{f}(k)$ , one must still show that

1) The contour integration may be interchanged with the two integrations over  $\mathbf{r}$  and  $\mathbf{r}'$  in eq. (11.222)

2) As  $A \rightarrow \infty$ , the contribution from the semi-circle vanishes.

The first point amounts to proving that the integral (11.220) converges uniformly with respect to  $\zeta$  on  $C$ . The second point requires an analysis of the asymptotic behaviour of  $G^{(+)}(\mathbf{r}, \mathbf{r}', \zeta)$  with respect to  $\zeta$ . The arguments are given in detail by Klein and Zemach [57] and will not be developed here. We then have

$$\tilde{f}(k) = \sum_{i=1}^N \frac{R_i}{k^2 - \zeta_i^2} + \frac{2}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty \frac{k' \operatorname{Im} \tilde{f}(k')}{k'^2 - (k + i\varepsilon)^2} dk' \quad (11.224)$$

where we have used the symmetry relation (11.214). Going back to the scattering amplitude  $f(k)$  we find that it satisfies the forward dispersion relation with *one* subtraction

$$f(k) = f_{B1} + \sum_{i=1}^N \frac{R_i}{k^2 - \zeta_i^2} + \frac{2}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty \frac{k' \operatorname{Im} f(k')}{k'^2 - (k + i\varepsilon)^2} dk' \quad (11.225)$$

where we have used the fact that  $\operatorname{Im} \tilde{f} = \operatorname{Im} f$  since  $f_{B1}$  is real. The conditions on the potential which are necessary to obtain this result have been given by Klein and Zemach [57]. Defining

$$I_v(\mathbf{r}) = \int \frac{|V(\mathbf{r}')|}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \quad (11.226)$$

they find that  $I_v(\mathbf{r})$  must be such that

$$\begin{aligned} I_v(\mathbf{r}) &< \infty \text{ for all } \mathbf{r} \\ I_v(\mathbf{r}) &\text{ is continuous in } \mathbf{r} \\ I_v(\mathbf{r}) &\sim \mathcal{O}(r^{-1}) \text{ as } r \rightarrow \infty. \end{aligned} \quad (11.227)$$

It is interesting to rewrite the dispersion relation (11.225) in terms of the energy  $E = \hbar^2 k^2 / 2m$  instead of the wave number  $k$ . Then

$$f(E) = f_{B1} + \sum_{i=1}^N \frac{\tilde{R}_i}{E - E_i} + \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty \frac{\operatorname{Im} f(E')}{E' - E - i\varepsilon} dE' \quad (11.228)$$

where  $E_i$  are the bound state energies and  $\tilde{R}_i$  the corresponding "residues". This form of the dispersion relation is valid for all values of  $E$  on the *physical* sheet of the complex  $E$ -plane. It must be remembered here that the *entire* physical sheet of the  $E$ -plane corresponds to the upper half  $k$ -plane  $\text{Im } k \geq 0$ . We also recall that the total Green's function  $G^{(+)}(\mathbf{r}, \mathbf{r}', E)$  is analytic in the  $E$ -plane except for bound state poles at  $E = E_i < 0$  and a cut extending along the positive real axis, which corresponds to the scattering states.

Let us now concentrate on real values of  $E$ . Using the relation (11.167) in (11.228), and remembering that  $f_{B1}$  and  $\tilde{R}_i$  are both real, we find that the real part of eq. (11.228) yields

$$\text{Re } f(E) = f_{B1} + \sum_{i=1}^N \frac{\tilde{R}_i}{E - E_i} + \frac{P}{\pi} \int_0^\infty \frac{\text{Im } f(E')}{E' - E} dE' \quad (11.229)$$

while the imaginary part reduces to the identity  $\text{Im } f = \text{Im } f$ . We may now use the optical theorem

$$\text{Im } f(E') = \frac{(2mE')^{1/2}/\hbar}{4\pi} \sigma_{\text{tot}}(E') \quad (11.230)$$

to express the integral on the right-hand side of eq. (11.229) in terms of the total cross section  $\sigma_{\text{tot}}(E')$ . Hence eqs. (11.229)–(11.230) allow one to calculate the forward scattering amplitude  $f(E)$  for any energy if the total cross section is known for all energies and the bound state energies  $E_i$  with the corresponding residues [63] are known. This is the most important consequence of the dispersion relation (11.229).

We now consider briefly dispersion relations for *nonforward scattering*. It is convenient to use the energy  $E$  and the wave vector transfer  $\Delta$  as variables to describe the scattering amplitude. We shall actually hold  $\Delta$  fixed to obtain a dispersion relation in the energy. Defining the vector

$$\mathbf{q} = \frac{1}{2}(\mathbf{k}_i + \mathbf{k}_f) \quad (11.231)$$

so that

$$q^2 = k^2 - \frac{1}{4}\Delta^2 = 2mE/\hbar^2 - \frac{1}{4}\Delta^2 \quad (11.232)$$

we may write the scattering amplitude as

$$f(E, \Delta) = f_{B1}(\Delta) - \frac{1}{4\pi} \int d\mathbf{r} d\mathbf{r}' \exp\{\frac{1}{2}i\Delta \cdot (\mathbf{r} + \mathbf{r}')\} \\ \times U(\mathbf{r})G^{(+)}(\mathbf{r}, \mathbf{r}', E)U(\mathbf{r}') \exp\{i\mathbf{q} \cdot (\mathbf{r}' - \mathbf{r})\} \quad (11.233)$$

where we have used the fact that the potential is spherically symmetric to deduce that the scattering amplitude does not depend on the direction of  $\Delta$ . For the same reason the vector  $\mathbf{q}$  can only appear as  $q^2$  so that there is no branch point at  $q = (k^2 - \frac{1}{4}\Delta^2)^{1/2}$ .

It is important to note that the integral on the right-hand side of eq. (11.233) does not exist for arbitrarily large  $\Delta$  at fixed  $k$ , since in this case  $q^2$

becomes negative and  $\exp[i(k^2 - \frac{1}{4}\Delta^2)^{1/2} \hat{q} \cdot (\mathbf{r}' - \mathbf{r})]$  increases exponentially. This difficulty, which arises in the "unphysical region" ( $\Delta > 2k$ ) may be avoided by requiring that [57]

$$\int d\mathbf{r} e^{i\mu r} U(r) < \infty, \quad \mu > 0 \quad (11.234)$$

in which case one obtains the dispersion relation

$$f(E, \Delta) = f_{B1}(\Delta) + \sum_{i=1}^N \frac{\tilde{R}_i(\Delta)}{E - E_i} + \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty \frac{\text{Im } f(E', \Delta)}{E' - E - i\varepsilon} dE' \quad (11.235)$$

valid for  $\Delta < 2\mu$ . We note that the evaluation of the integral on the right-hand side of eq. (11.235) requires the knowledge of  $\text{Im } f(E', \Delta)$  down to  $E' = 0$ . However, for  $\Delta \neq 0$  fixed, the region  $0 \leq E' < \hbar^2 \Delta^2 / 8m$  corresponds to an *unphysical* region of the scattering amplitude, for which  $\text{Im } f(E', \Delta)$  cannot be extracted from experiments. What we need then is the analytic continuation of  $\text{Im } f(E', \Delta)$  into this unphysical region. The simplest approach to this problem is to use the partial wave expansion

$$f = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp\{i\delta_l(k)\} \sin \delta_l(k) P_l\left(1 - \frac{\Delta^2}{2k^2}\right). \quad (11.236)$$

Except for pathological cases, this series converges in the physical region, for which

$$-1 \leq \omega \leq 1 \quad (11.237)$$

where we have defined  $\omega = 1 - \Delta^2/(2k^2)$ . Here, however, we need to examine the convergence of the series (11.236) when  $k^2 \rightarrow 0$ , i.e. for  $\omega \rightarrow -\infty$ . To accomplish this, we use a well known theorem of analysis [see e.g. 64] which states that if a function of  $\omega = \cos \theta$  is analytic inside an ellipse in the complex  $\omega$ -plane with foci at  $\pm 1$ , then this function may be expanded in a convergent series of Legendre polynomials inside that ellipse. It is possible to show [see e.g. 65] that  $\text{Im } f(E, \theta)$  is indeed analytic inside an ellipse with foci at  $\omega = \pm 1$ , semimajor axis  $1 + 2\mu^2/k^2$  and semiminor axis  $(2\mu/k)(1 + \mu^2/k^2)^{1/2}$ . We may then use the above theorem to carry out the analytic continuation of  $\text{Im } f$  for real values of  $\omega = \cos \theta$  such that

$$|\omega| < 1 + 2\mu^2/k^2 \quad (11.238)$$

or

$$\Delta^2 < 4k^2 + 4\mu^2. \quad (11.239)$$

Since we are interested in continuing  $\text{Im } f(E, \Delta)$  down to  $E = 0$  (i.e.  $k = 0$ ), we see that the required condition of analytic continuation of  $\text{Im } f(E, \Delta)$  into this unphysical region by means of the series (11.236) is

$$\Delta < 2\mu. \quad (11.240)$$

This is precisely the range of  $\Delta$  for which the dispersion relation (11.235) at fixed momentum transfer holds. Hence no further restriction is required

for the analytic continuation of  $\text{Im } f(E, \Delta)$  into the unphysical region than for the derivation of the dispersion relation (11.235) itself.

An interesting question is to ask whether the non-forward dispersion relation (11.235) together with the unitarity condition (4.94), namely

$$\text{Im } f(\mathbf{k}_i, \mathbf{k}_f) = \frac{k}{4\pi} \int f^*(\mathbf{k}_f, \mathbf{k}') f(\mathbf{k}_i, \mathbf{k}') d\Omega' \quad (11.241)$$

may provide the basis of a dynamical theory, i.e. an alternative to the Schrödinger equation. The answer is negative because of the limitation  $\Delta < 2\mu$  on the wave vector transfers. It is therefore of great interest to investigate whether the dispersion relation can be extended to larger values of  $\Delta$  and also to inquire into the analytic properties of  $f(E, \Delta)$  with respect to  $\Delta$ . This was first studied by Mandelstam [66] in connection with the analysis of pion-nucleon scattering. He conjectured a double dispersion representation that exhibits the analytic properties of the scattering amplitude as a function of both the energy and the momentum transfer.

The Mandelstam representation has attracted considerable interest in strong interaction physics [67] although the problem of its derivation has not yet been solved. For non-relativistic potential scattering, however, the Mandelstam representation may be derived. We shall not discuss here these calculations which may be found in the literature [68].

#### 11.5.4. Dispersion relations for the Jost function

We have shown in Section 11.1 that the Jost function  $f_l(k)$  is analytic in the lower half-plane and that  $f_l(k) - 1$  tends to zero as  $|k| \rightarrow \infty$  and  $\text{Im } k \leq 0$ . We may then apply Cauchy's theorem to write

$$f_l(k) - 1 = \frac{1}{2\pi i} \oint_C \frac{f_l(k') - 1}{k' - k} dk' \quad (11.242)$$

where  $C$  is the contour shown on Fig. 11.10 and containing the point  $k$ . Letting the radius of the semi-circle tend to infinity, we obtain

$$f_l(k) = 1 - \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{f_l(k') - 1}{k' - k} dk' \quad (11.243)$$

since the contribution from the semi-circle vanishes. If we let  $k$  approach the real axis from below, we may write

$$f_l(k) = 1 - \frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{f_l(k') - 1}{k' - (k - i\varepsilon)} dk' \quad (11.244)$$

which, by using eq. (11.167) yields

$$f_l(k) = 1 - \frac{P}{i\pi} \int_{-\infty}^{+\infty} \frac{f_l(k') - 1}{k' - k} dk'. \quad (11.245)$$



Taking the real part of this equation, we obtain the *dispersion relation*

$$\operatorname{Re} f_l(k) = 1 - \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Im} f_l(k')}{k' - k} dk' \quad (11.246)$$

or, using again eq. (11.167)

$$f_l(k) = 1 - \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{\operatorname{Im} f_l(k')}{k' - k + i\varepsilon} dk'. \quad (11.247)$$

Because  $f_l(k) = |f_l(k)| \exp[i\delta_l(k)]$  we may also write

$$f_l(k) = 1 - \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{f_l(k') \exp\{-i\delta_l(k')\} \sin \delta_l(k')}{k' - k + i\varepsilon} dk'. \quad (11.248)$$

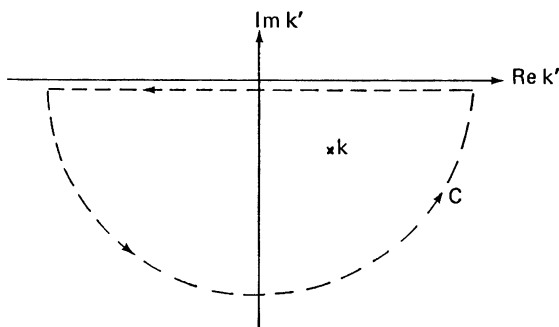


Fig. 11.10. Illustration of the contour  $C$  of the text.

The solution of this integral equation for  $f_l(k)$  requires in general the knowledge of the zeros of  $f_l(k)$  in the lower half  $k$ -plane (i.e. the bound state energies  $E_l$ ) in addition to the phase shift  $\delta_l(k)$ . It is then possible to show [14, 69] that

$$f_l(k) = \prod_{i=1}^{n_l} \left(1 - \frac{E_i}{E}\right) \exp \left[ -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\delta_l(k')}{k' - k + i\varepsilon} dk' \right] \quad (11.249)$$

where  $n_l$  is the number of bound states of angular momentum  $l$  and  $E = \hbar^2 k^2 / 2m$ .

It is also of interest to obtain dispersion relations for the Jost function in the *energy* plane. To this end, we first note that

$$f_l(-k) = 1 + \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{(k' + k) \operatorname{Im} f_l(-k')}{k'^2 - (k + i\varepsilon)^2} dk'. \quad (11.250)$$

Defining  $D_l(E) \equiv f_l(-k)$ , we obtain

$$D_l(E) = 1 + \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_0^{\infty} \frac{\operatorname{Im} D_l(E')}{E' - E - i\varepsilon} dE' \quad (11.251)$$

where we have used the fact that  $\operatorname{Im} f_l(k)$  is an odd function of  $k$  [because  $f_l(k) = f_l^*(-k)$ ]. We note that the physical value of  $D_l(E)$  is obtained by

approaching the real axis from above. The representation (11.251) allows one to extend  $D_l(E)$  as an analytic function in the entire physical sheet of the complex energy plane, cut along the real positive axis. From the definition of  $D_l(E)$  we see that along the real axis

$$D_l(E) = |D_l(E)| \exp\{-i\delta_l(E)\} \quad (11.252)$$

so that

$$\lim_{\varepsilon \rightarrow 0^+} \frac{D_l(E + i\varepsilon)}{D_l(E - i\varepsilon)} = \exp\{-2i\delta_l(E)\} = S_l^{-1}(E). \quad (11.253)$$

We also obtain from eq. (11.249) the expression

$$D_l(E) = \prod_{i=1}^n \left(1 - \frac{E_i}{E}\right) \exp \left[ -\frac{1}{\pi} \int_0^\infty \frac{\delta_l(E')}{E' - E + i\varepsilon} dE' \right] \quad (11.254)$$

where we have used the fact that  $\delta_l(k)$  is odd in  $k$ .

## 11.6. Effective range theory

In this section we want to apply our knowledge of the analytic properties of scattering amplitudes to the analysis of potential scattering at *low energies*. We shall first prove by using the properties of the Jost functions that for a certain class of potentials the quantity  $k^{2l+1} \cot \delta_l(k)$  may be expanded for sufficiently small values of  $k$  as a power series in  $k^2$ .

To this end, let us consider the partial wave amplitudes

$$a_l(k) = \frac{1}{2ik} [S_l(k) - 1] \quad (11.255)$$

which we express in terms of the Jost functions  $f_l(k)$  and  $f_l(-k)$  [see eq. (11.93)] as

$$a_l(k) = \frac{1}{2ik} \left[ \frac{f_l(k) - f_l(-k)}{f_l(-k)} \right]. \quad (11.256)$$

We impose on the potential the condition (11.21), namely

$$\int_0^\infty e^{\mu r} |U(r)| dr < \infty$$

so that the Jost function  $f_l(k)$  is analytic for  $\text{Im } k < \frac{1}{2}\mu$  and the partial wave amplitude  $a_l(k)$  may be continued off the real axis into the complex  $k$ -plane.

Following Goldberger and Watson [70], we rewrite eq. (11.256) in the *energy plane* as

$$a_l(E) = N_l(E)/D_l(E) \quad (11.257)$$

where  $D_l(E) \equiv f_l(-k)$  as in the preceding section and

$$N_l(E) = \frac{f_l(k) - f_l(-k)}{2ik}. \quad (11.258)$$

We note that since  $f_l^*(-k^*) = f_l(k)$  the function  $N_l(E)$  is real for real  $E$ . Furthermore  $N_l(E)$  is unmodified when  $k \rightarrow -k$ . Thus, since  $f_l(k)$  is analytic in the  $k$ -plane for  $\text{Im } k < \frac{1}{2}\mu$ ,  $N_l(E)$  is analytic in the energy plane for

$$|E| < \hbar^2 \mu^2 / 8m. \quad (11.259)$$

Let us now consider the quantity

$$a_l^{-1}(E) = D_l(E)/N_l(E) = k \cot \delta_l(k) - ik. \quad (11.260)$$

Using the fact that  $N_l(E)$  is real [71], we have

$$kN_l(E) \cot \delta_l(E) = D_l(E) + ikN_l(E). \quad (11.261)$$

Now  $N_l(E)$  is an analytic function of  $E$  inside the circle defined by (11.259) and  $D_l(E)$ , as given by eq. (11.251), is analytic in the  $E$ -plane cut along the real axis. Moreover, as  $E \rightarrow E \exp(2i\pi)$ , we see that

$$\begin{aligned} D_l(E) &\rightarrow D_l(E e^{2i\pi}) = f_l(k) \\ &= f_l(-k) + [f_l(k) - f_l(-k)] = D_l(E) + 2ikN_l(E) \end{aligned} \quad (11.262)$$

while at the same time  $ikN_l(E) \rightarrow -ikN_l(E)$ . Therefore, the right-hand side of eq. (11.261) is unchanged when  $E \rightarrow E \exp(2i\pi)$  and we may conclude that the function  $kN_l(E) \cot \delta_l(E)$  is *analytic in the  $E$ -plane within a circle of radius  $\hbar^2 \mu^2 / 8m$* . We may thus write in this domain the power series expansion

$$kN_l(E) \cot \delta_l(E) = \alpha_0 + \alpha_1 E + \alpha_2 E^2 + \dots \quad (11.263)$$

Except for a zero-energy resonance [in which case  $D_l(0) = 0$ ], we see from eq. (11.257) that for  $|E| < \hbar^2 \mu^2 / 8m$  we may also expand the function  $N_l(E)$  as

$$N_l(E) = k^{2l}(\beta_0 + \beta_1 E + \beta_2 E^2 + \dots) \quad (11.264)$$

where we have used the fact [see eq. (4.124)] that

$$a_l(k) \underset{k \rightarrow 0}{\sim} k^{2l}. \quad (11.265)$$

Replacing the development (11.264) in eq. (11.263), we find that

$$k^{2l+1} \cot \delta_l(E) = c_0 + c_1 E + c_2 E^2 + \dots \quad (11.266)$$

for  $|E| < \hbar^2 \mu^2 / 8m$ . We have therefore proved our statement about the analyticity of the quantity  $k^{2l+1} \cot \delta_l$  as a function of  $E$  (or  $k^2$ ), provided the potential obeys the condition (11.21).

Let us now determine the first coefficients of the expansion (11.266). We start from the radial equation (4.17), namely

$$[d^2/dr^2 + k^2 - l(l+1)/r^2 - U(r)]u_l(k, r) = 0 \quad (11.267)$$

and shall only analyze in detail the case of s-wave scattering. We denote by  $u^0(r)$  the solution of this equation for  $k \rightarrow 0$  and  $l = 0$ . That is

$$u^0(r) \equiv \lim_{k \rightarrow 0} u_0(k, r). \quad (11.268)$$

Therefore

$$[d^2/dr^2 - U(r)]u^0(r) = 0. \quad (11.269)$$

In the region  $r \gg a$ , where the potential can be neglected [72], we have

$$\frac{d^2}{dr^2} u^0(r) \simeq 0 \quad (11.270)$$

and therefore [73]

$$u^0(r) \simeq Br + C, \quad r \gg a. \quad (11.271)$$

On the other hand, from eq. (4.44), we deduce that

$$u^0(r) \xrightarrow{r \rightarrow \infty} A[r - \alpha] \quad (11.272)$$

where

$$\alpha = - \lim_{k \rightarrow 0} \frac{\tan \delta_0(k)}{k} \quad (11.273)$$

is the *scattering length* defined by eq. (4.125). Thus  $\alpha$  has a simple geometrical meaning: it is the intersection of the asymptote to  $u^0(r)$  with the  $r$  axis (see Fig. 11.11). From eq. (11.269) and this geometrical interpretation of  $\alpha$  one immediately deduces that

- 1) For a repulsive potential ( $U > 0$ ) the curvature of  $u^0$  is always away from the  $r$ -axis so that  $\alpha > 0$ .
- 2) For an attractive potential
  - a) incapable of producing an s-wave bound state:  $\alpha < 0$  (see Fig. 11.12a),
  - b) capable of producing an s-wave virtual state or "zero-energy resonance":  $\alpha = \infty$  (see Fig. 11.12b),
  - c) capable of producing one s-wave bound state:  $\alpha > 0$  (see Fig. 11.12c).

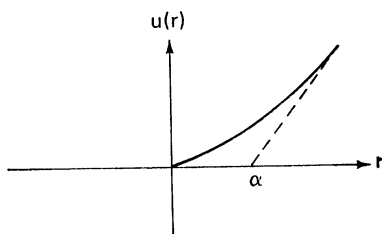


Fig. 11.11. Illustration of the geometrical meaning of the scattering length  $\alpha$ .

These considerations can easily be generalized to the case of several bound states.

Returning to the definition (11.273), we note that

$$\lim_{k \rightarrow 0} k \cot \delta_0(k) = -\frac{1}{\alpha} \quad (11.274)$$

so that the first coefficient  $c_0$  of the expansion (11.266) (for  $l = 0$ ) is given by  $c_0 = -\alpha^{-1}$ .

To determine the next coefficient, we consider again the radial equation (11.267) for two arbitrary energies

$$E_1 = \hbar^2 k_1^2 / 2m; \quad E_2 = \hbar^2 k_2^2 / 2m \quad (11.275)$$

and we define

$$u^1(r) \equiv u_0(k_1, r); \quad u^2(r) \equiv u_0(k_2, r). \quad (11.276)$$

Hence

$$[d^2/dr^2 + k_1^2 - U(r)]u^1(r) = 0 \quad (11.277)$$

and

$$[d^2/dr^2 + k_2^2 - U(r)]u^2(r) = 0. \quad (11.278)$$

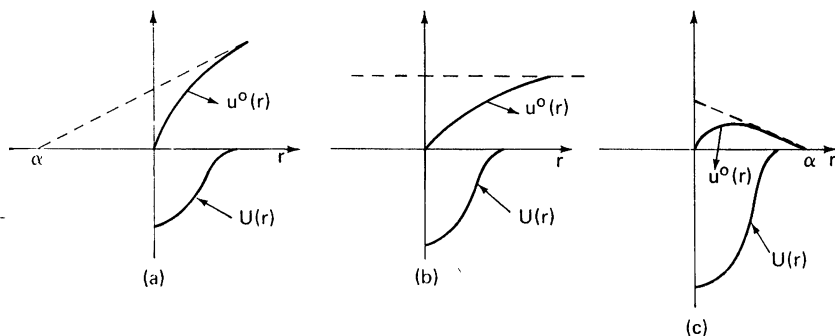


Fig. 11.12. Illustration of the scattering length  $\alpha$  for various attractive potentials.

If we multiply eq. (11.277) by  $u^2(r)$ , eq. (11.278) by  $u^1(r)$ , and subtract, we obtain

$$\frac{d}{dr}(u^1 u^{2'} - u^2 u^{1'}) = (k_1^2 - k_2^2) u^1 u^2 \quad (11.279)$$

where the prime denotes differentiation with respect to  $r$ .

Let us now define two functions  $v^1$  and  $v^2$ , solutions of the radial equation without the potential,

$$\begin{aligned} [d^2/dr^2 + k_1^2]v^1(r) &= 0, \\ [d^2/dr^2 + k_2^2]v^2(r) &= 0 \end{aligned} \quad (11.280)$$

so that one has

$$\lim_{r \rightarrow \infty} u^i(r) = v^i(r). \quad (11.281)$$

Let us choose our “normalization” such that  $v^i(0) = 1$  ( $i = 1, 2$ ). Thus

$$v^i(r) = \frac{\sin(k_i r + \delta_0)}{\sin \delta_0}. \quad (11.282)$$

We also have

$$\frac{d}{dr}(v^1 v^{2'} - v^2 v^{1'}) = (k_1^2 - k_2^2) v^1 v^2. \quad (11.283)$$

Subtracting (11.283) from (11.279) and integrating on  $r$  from 0 to  $\infty$ , we obtain

$$[u^1 u^{2'} - u^2 u^{1'} - v^1 v^{2'} + v^2 v^{1'}]_0^\infty = (k_1^2 - k_2^2) \int_0^\infty (u^1 u^2 - v^1 v^2) dr. \quad (11.284)$$

Taking into account eq. (11.282) and the boundary conditions, we then have

$$k_1 \cot \delta_0(k_1) - k_2 \cot \delta_0(k_2) = (k_1^2 - k_2^2) \int_0^\infty (v^1 v^2 - u^1 u^2) dr. \quad (11.285)$$

For the particular case  $k_1 = k$  and  $k_2 \rightarrow 0$ , this equation becomes

$$k \cot \delta_0(k) = -\frac{1}{\alpha} + k^2 \int_0^\infty (v^k v^0 - u^k u^0) dr \quad (11.286)$$

with

$$v^0(r) = 1 - r/\alpha \quad (11.287)$$

and  $v^k \equiv v^1$ ,  $u^k \equiv u^1$  for  $k_1 = k$ .

Let us define the quantity

$$b(k) = 2 \int_0^\infty (v^k v^0 - u^k u^0) dr. \quad (11.288)$$

We may then rewrite eq. (11.286) as

$$k \cot \delta_0(k) = -\frac{1}{\alpha} + \frac{1}{2} b(k) k^2 \quad (11.289)$$

which is known as *Bethe's formula* [74]. It is important to note that the potential  $U(r)$  should tend sufficiently fast to zero as  $r \rightarrow \infty$  so that the integral on the right-hand side of eqs. (11.284) or (11.288) exists. The analysis made at the beginning of this section shows that the condition (11.21) on the potential is sufficient for our purposes. For such potentials, the contribution to the integral on the right-hand side of eq. (11.288) arises essentially from the "internal" region (within the "range" of the potential), where one may replace [75] approximately  $u^k$  by  $u^0$  and  $v^k$  by  $v^0$ . Then eq. (11.289) becomes the *effective range formula*

$$k \cot \delta_0(k) = -\frac{1}{\alpha} + \frac{1}{2} r_e k^2 + \dots \quad (11.290)$$

where the *effective range*  $r_e$  is defined by

$$r_e = 2 \int_0^\infty [(v^0)^2 - (u^0)^2] dr. \quad (11.291)$$

The factor of two in front of the integral has been chosen in such a way that for a square well potential of range  $a$  one has  $r_e = a$ . We have thus determined the second coefficient of the expansion (11.266) when  $l = 0$ .

The effective range formula (11.290) has been particularly useful to analyze nucleon-nucleon scattering at low energies. The existence of a

formula of the type (11.266) was first realized empirically by Breit et al. [76], then discussed by Landau and Smorodinsky [77] and demonstrated from the variational method (see Section 10.2) by Schwinger [78]. The simpler derivation given here is based on the work of Chew and Goldberger [79], Barker and Peierls [80], and Bethe [74]. We note that from eq. (11.290) we obtain for the total cross section at low energies

$$\sigma_{\text{tot}} \simeq \sigma_0 \simeq \frac{4\pi}{k^2 + [-1/\alpha + \frac{1}{2}r_e k^2]^2} \quad (11.292)$$

which of course reduces to  $4\pi\alpha^2$  when  $k \rightarrow 0$ .

The effective range theory also permits one to establish a relationship between the effective range  $r_e$  and  $l = 0$  bound states, if they exist. Indeed, let us consider the case where  $k_1^2 = k^2 > 0$  but  $k_2^2 = -v^2 < 0$  (so that the bound state energy is  $E_B = -\hbar^2 v^2/2m$ ). Then, from eq. (11.285), we have

$$k \cot \delta_0(k) + |v| = (k^2 + v^2) \int_0^\infty (v^k v^v - u^k u^v) dr \quad (11.293)$$

where

$$[d^2/dr^2 - v^2]v^v(r) = 0 \quad (11.294)$$

and

$$[d^2/dr^2 - v^2 - U(r)]u^v(r) = 0. \quad (11.295)$$

For a bound state of small binding energy ( $v \rightarrow 0$ ), the relation (11.293) becomes

$$k \cot \delta_0(k) + |v| = \frac{1}{2}r_e(k^2 + v^2) \quad (11.296)$$

and for  $k \rightarrow 0$ , one has

$$-1/\alpha = -|v| + \frac{1}{2}r_e v^2. \quad (11.297)$$

The equations (11.296) and (11.297) permit one to express the effective range as a function of the energy of the bound state (since  $|v| = [2m|E_B|/\hbar^2]^{1/2}$ ), provided  $\delta_0(k)$  or  $\alpha$  are known with sufficient precision.

As an application of these considerations, let us examine low-energy ( $l = 0$ ) neutron-proton scattering in the C.M. system. Because the nuclear forces are spin-dependent, we must consider both singlet ( $S = 0$ ) and triplet ( $S = 1$ ) scattering. For singlet scattering we shall use the symbols  $\alpha^s$ ,  $r_e^s$  and  $\sigma^s$  while for triplet scattering we write  $\alpha^t$ ,  $r_e^t$  and  $\sigma^t$ . Since the deuteron bound state occurs for  $S = 1$ , we use eq. (11.297) in this case to obtain

$$-1/\alpha^t \simeq -|v| + \frac{1}{2}r_e^t v^2. \quad (11.298)$$

Here

$$|v| = (M|E_B|/\hbar^2)^{1/2} \quad (11.299)$$

where  $M$  is the nucleon mass [81] and  $|E_B| = 2.23$  MeV is the deuteron binding energy. If the initial spins are randomly distributed, the total cross section for the observed process is given by

$$\sigma = \frac{1}{4}\sigma^s + \frac{3}{4}\sigma^t. \quad (11.300)$$

The experimental data then yield [82]  $\alpha^s = -2.4 \times 10^{-12}$  cm,  $\alpha^t = 5.4 \times 10^{-13}$  cm,  $r_e^s = 2.5 \times 10^{-13}$  cm and  $r_e^t = 1.7 \times 10^{-13}$  cm. Had we neglected the spin dependence of nuclear forces, we would have obtained from eq. (11.297) a (single) scattering length  $\alpha = 5.4 \times 10^{-13}$  cm yielding a total cross section in strong disagreement with experiment. The suggestion that spin-dependent effects must play an important role in nucleon–nucleon interactions was made by Wigner in 1935.

It is also possible to develop the effective range theory in the presence of a Coulomb potential [see e.g. 83]. An important application is the study of low-energy proton–proton scattering which, in particular, allows one to test the postulate of *charge independence*. According to this postulate, the interaction between two nucleons is the same (for a given state of angular momentum and spin) whether the particles are neutrons or protons.

To conclude this section on the effective range theory, we mention the, case of a potential which does *not* obey the condition (11.21) and for which therefore, we should not expect an expansion of the form (11.266) to be valid. This is the *polarization potential*

$$V(r) = -\bar{\alpha}Q^2/2(r^2 + d^2)^2 \quad (11.301)$$

which plays an important role in the scattering of a charged particle by a neutral atom [84]. Here  $Q$  is the charge of the incident particle,  $\bar{\alpha}$  is the polarizability of the atom and  $d$  is a parameter having the dimensions of a length. We note that this interaction behaves like  $r^{-4}$  for large  $r$ . Although the effective range integral (11.291) diverges in this case (Problem II, 61), a modified expansion of the type

$$k \cot \delta_0(k) = -\frac{1}{\alpha} + \frac{\pi P^2}{3\alpha^2}k + \mathcal{O}\left(\frac{P^2 k^2}{\alpha} \log Pk\right) \quad (11.302)$$

has been obtained by O'Malley, Spruch and Rosenberg [85]. Here  $\alpha$  is the scattering length and

$$P^2 = \bar{\alpha}mQ^2/\hbar^2. \quad (11.303)$$

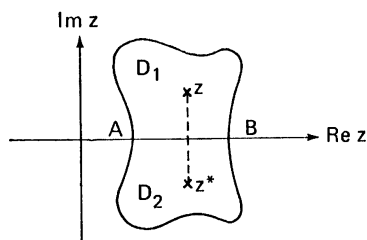
We observe that the long range of the potential introduces a term linear in  $k$  and a term of the form  $k^2 \log k$ . This modified effective range expansion has been useful in describing the low-energy scattering of a charged particle by a neutral atom.

## References and notes

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 [8] POINCARÉ, H. (1884), Acta Math. **4**, 201.  
 [9] Let  $f_1(z)$  be an analytic function in the domain  $D_1$  which takes on real values on the part AB of the real axis Re  $z$  (see figure). The *Schwarz reflection principle* states that



the analytic continuation of  $f_1(z)$  in the domain  $D_2$  (considered as the image of  $D_1$  through the mirror AB) is given by  $f_2(z) = f_1^*(z^*)$ .

- [10] BARGMANN, V. (1949), Rev. Mod. Phys. **21**, 488.  
 [11] The Wronskian of two functions  $f$  and  $g$  is defined as  $W[f, g] = fg' - f'g$ . In the text, the differentiation is with respect to the variable  $r$ .  
 [12] Exceptions may occur for "pathological" potentials which do not satisfy the conditions (11.2) and (11.3) and where  $f(0) = 0$  can correspond to a bound state with  $l = 0$ . See for example NEWTON, R. G. (1966), *Scattering Theory of Waves and Particles* (McGraw-Hill, New York) Section 14.7.  
 [13] For higher angular momenta ( $l \geq 1$ ), the point  $k = 0$  may correspond to a bound state. See NEWTON, loc. cit [12] Section 12.2.  
 [14] NEWTON, R. G. (1960), J. Math. Phys. **1**, 319.  
 [15] If  $g(z) = (z - z_0)^n f(z)$  with  $f(z_0) \neq 0$  and  $n$  is a positive integer, then  $z = z_0$  is a zero of order  $n$  of  $g(z)$ . If  $n = 1$ , this zero is called simple.  
 [16] BARGMANN, V. (1952), Proc. Natl. Acad. Sci. U.S. **38**, 961.  
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 [18] The unitary character of the  $S$  matrix is seen here to depend on the fact that the phase shifts are real. This is the case because we are presently dealing with a simple potential scattering problem. We shall prove in Part III that the unitary property of the  $S$  matrix is a very general one, being a result of the conservation of probability.  
 [19] The concept of enhancement factor, introduced by E. Fermi, has been useful in the analysis of various elementary particle collisions, particularly in connection with the theory of final state interactions. We shall return to this subject in Chapter 21.  
 [20] Indeed, the numerator  $f(k)$  of eq. (11.72) cannot vanish at the same points as the denominator  $f(-k)$  because of eqs. (11.36) and (11.37).  
 [21] MA, S. T. (1947), Phys. Rev. **71**, 195.  
 [22] The apparent singularity at  $k = 0$  is spurious because  $a_l$  tends to zero as  $k^{2l}$ . [Except when  $a_l = -(l + 1)$ , see Section 4.3.3.]  
 [23] We recall the argument theorem: Let  $f(z)$  be analytic inside and on a simple closed curve  $C$  except for a finite number of poles inside  $C$ . Assume that  $f(z) \neq 0$  on  $C$ . Then, if  $N$  and  $P$  are respectively the number of zeros and poles of  $f(z)$  inside  $C$ , including the multiplicities, one has
- $$\frac{1}{2\pi i} \oint_C \frac{f'(z)}{f(z)} dz = N - P.$$
- [24] It is unnecessary to write  $\delta_l(0) = (n_l + 1)\pi$  since - in contrast to the case  $l = 0$  - the possible zero of  $f_l(k)$  at  $k = 0$  corresponds for  $l \geq 1$  to a genuine bound state leading to a square integrable eigenfunction. It is therefore included in  $n_l$ .

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- [29] OMNÈS, R. L. (1966), *Ann. Rev. Nucl. Sci.* **16**, 263.
- [30] We shall assume that the function  $\rho(\nu)$  which appears in eq. (11.116) is bounded everywhere except perhaps for delta-function singularities. The two inequalities (11.2) and (11.3) imply that  $\rho(\nu)/\nu \rightarrow 0$  as  $\nu \rightarrow 0$  and that  $\rho(\nu) \rightarrow 0$  as  $\nu \rightarrow \infty$ . Furthermore, the fact that  $\nu_0 > 0$  in eq. (11.116) means that  $U(r)$  has a range  $\nu_0^{-1}$  such that the inequality (11.21) is satisfied for  $0 < \mu \leq \nu_0$ .
- [31] We note that  $\tilde{f}(l, -k)$  cannot vanish for  $\text{Im } \lambda = 0$ , since in that case  $\tilde{f}(l, k)$  would also vanish. Then, using eq. (11.50), we would deduce that  $\phi = 0$ , in contradiction with the boundary condition (11.117).
- [32] Meromorphic functions are analytic functions except for poles.
- [33] The idea of replacing an infinite series by a contour integral of an analytic function was first introduced by  
POINCARÉ, H. (1910), *Rend. Circ. Mat. Palermo* **29**, 169 and  
NICHOLSON, J. W. (1910), *Phil. Mag.* **19**, 516.  
See also  
WATSON, G. N. (1918), *Proc. Roy. Soc. (London)* **95**, 83;  
SOMMERFELD, A. (1949), *Partial Differential Equations of Physics* (Academic Press, New York) p. 282.
- [34] Bateman Manuscript Project (1953), *Higher Transcendental Functions*, ed. A. Erdelyi (McGraw-Hill, New York) p. 122.
- [35] For example, if  $S$  is a given interpolation of the  $S$ -matrix element, we may replace it by  $S' = S + f \sin \pi l$ , where  $f$  is an arbitrary function of  $l$  which is finite at integer values of  $l$ .
- [36] We follow here the treatment of SVENSSON, B. E. Y. (1967), in *Proc. 1967 CERN School of Physics*, Vol. II, CERN Report 67-24.
- [37] This is always satisfied for positive energies, since then  $\text{Im } \alpha_i > 0$  as we have shown above.
- [38] Ref. [34] p. 170, eq. (7).
- [39] In contrast to the previous treatment, however, we analyze here directly the physical partial wave amplitude  $a_{l=m}(E)$  instead of considering the amplitude  $a(l, E)$  about the Regge pole  $l \simeq \alpha$  and extrapolating to the physical value of  $l$ .
- [40] Ref. [27] Chapter 15.
- [41] We recall that the problem of the non-relativistic scattering of two particles A and B of masses  $m_A$  and  $m_B$  which interact through a potential  $V(r)$  [where  $r$  is their relative coordinate] is equivalent, in the C.M. system, to the scattering of a particle of mass  $m = m_A m_B / (m_A + m_B)$  by the potential  $V(r)$ .
- [42] This is the case for example in nucleon-nucleon scattering.
- [43] This section is based on lectures by GOLDBERGER, M. L. (1961), in *Dispersion Relations and Elementary Particles* (Wiley, New York); see also  
GOLDBERGER, M. L. and K. M. WATSON, (1964) *Collision Theory* (Wiley, New York) Chapter 10;  
ROMAN, P. (1965), *Advanced Quantum Theory* (Addison-Wesley, Reading, Mass.) Chapter 3.
- [44] That is, the intensity decreases by  $\exp(-\alpha x)$  in a distance  $x$ .

- [45] Let  $f(x)$  be a continuous function for  $a \leq x \leq b$  except at the point  $x_0$  such that  $a < x_0 < b$ . One defines

$$\int_a^b f(x) dx = \lim_{\substack{\varepsilon_1 \rightarrow 0^+ \\ \varepsilon_2 \rightarrow 0^+}} \left[ \int_a^{x_0 - \varepsilon_1} f(x) dx + \int_{x_0 + \varepsilon_2}^b f(x) dx \right]. \quad (\text{I})$$

In certain cases this limit does not exist except when  $\varepsilon_1 = \varepsilon_2 = \varepsilon$ . The (Cauchy) principal value is then defined as

$$\text{P} \int_a^b f(x) dx = \lim_{\varepsilon \rightarrow 0^+} \left[ \int_a^{x_0 - \varepsilon} f(x) dx + \int_{x_0 + \varepsilon}^b f(x) dx \right]. \quad (\text{II})$$

For example  $\text{P} \int_{-1}^{+1} x^{-3} dx = 0$  while the corresponding limit (I) with  $\varepsilon_1 \neq \varepsilon_2$  and  $x_0 = 0$  does not exist.

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$$\lim_{\varepsilon \rightarrow 0^+} \int_a^b \frac{f(x)}{x - x_0 \mp i\varepsilon} dx = \text{P} \int_a^b \frac{f(x)}{x - x_0} dx \pm i\pi f(x_0)$$

where  $f(x)$  is regular in the neighbourhood of the real axis.

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## Time-Dependent Potential Scattering

We have already pointed out in Chapter 3 that the time-independent approach to scattering processes represents an idealization of the experimental situation. Indeed, it is obvious that the interaction between the “beam” and “target” particles only begins when the incident beam is sent on the target and stops when the scattered particle is detected. We shall study in this chapter how to take the time-dependence of the interaction into account in the simple case of potential scattering. A general time-dependent approach to collision phenomena will be developed in Part III.

We begin in Sections 12.1 and 12.2 by generalizing the methods of Chapter 5 to obtain the time-dependent Green’s functions and integral equations describing the collision process when the interaction  $V(\mathbf{r}, t)$  depends explicitly on the time variable. Section 12.3 is devoted to time-dependent perturbation theory. We first consider a method of solution of the dynamical equation which is analogous to the treatment given in Chapter 8; another perturbative approach, the method of “variation of the constants” will also be analyzed. In Section 12.4 we evaluate the transition probabilities and therefore the cross sections which (see Section 1.3) may be defined as transition probabilities per unit time, per scattering center and per unit incident flux.

### 12.1. Time-dependent Green’s functions [1]

Let us consider the non-relativistic scattering of a spinless particle of mass  $m$  by a time-dependent potential  $V(\mathbf{r}, t)$ . We shall treat this collision phenomenon as a modification of the (free) initial state of the particle caused by the interaction acting during a certain time interval and inducing *transitions* in the

system. We must therefore solve the *time-dependent* Schrödinger equation

$$H\Psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) \quad (12.1)$$

where the Hamiltonian operator, written in the coordinate representation, reads

$$H = -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}, t). \quad (12.2)$$

We shall also denote by

$$H_0 = -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 \quad (12.3)$$

the time-independent, “unperturbed” Hamiltonian such that

$$H_0 \Phi(\mathbf{r}) = E \Phi(\mathbf{r}). \quad (12.4)$$

The eigenstates of  $H_0$  are therefore given by

$$\Phi(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (12.5)$$

where  $E = \hbar^2 k^2 / 2m$  and we have adopted the “normalization” conventions of Section 5.1. The stationary solution of the time-dependent Schrödinger equation

$$\left[ i\hbar \frac{\partial}{\partial t} - H_0 \right] \varphi(\mathbf{r}, t) = 0 \quad (12.6)$$

corresponding to the energy  $E$  is therefore given by

$$\varphi(\mathbf{r}, t) = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \exp(-iEt/\hbar)$$

or

$$\varphi(\mathbf{r}, t) = (2\pi)^{-3/2} \exp\{i(\mathbf{k} \cdot \mathbf{r} - \omega t)\} \quad (12.7)$$

with  $\omega = E/\hbar$ .

Let us now return to the full time-dependent Schrödinger equation (12.1). As in Section 5.1, we first rewrite this equation as

$$\left[ i\hbar \frac{\partial}{\partial t} - H_0 \right] \Psi(\mathbf{r}, t) = V(\mathbf{r}, t) \Psi(\mathbf{r}, t) \quad (12.8)$$

where we consider again the right-hand side as an inhomogeneous term. The general solution of this equation may be written as

$$\Psi(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \int K_0(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \Psi(\mathbf{r}', t') d\mathbf{r}' dt' \quad (12.9)$$

where  $K_0(\mathbf{r}, t; \mathbf{r}', t')$  is a *time-dependent Green's function* or *propagator* [2] such that

$$\left[ i\hbar \frac{\partial}{\partial t} - H_0 \right] K_0(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}') \delta(t - t'). \quad (12.10)$$

In order to obtain the function  $K_0$  it is clearly sufficient to solve the equation

$$\left[ i\hbar \frac{\partial}{\partial \tau} + \frac{\hbar^2}{2m} \nabla_{\mathbf{R}}^2 \right] K_0(\mathbf{R}, \tau) = \delta(\mathbf{R})\delta(\tau) \quad (12.11)$$

where we have set  $\mathbf{R} = \mathbf{r} - \mathbf{r}'$  and  $\tau = t - t'$ . As in Section 5.2, it is convenient to study this equation in wave vector space. We first note that

$$\delta(\mathbf{R})\delta(\tau) = (2\pi)^{-4} \int \exp(i\mathbf{k}' \cdot \mathbf{R}) e^{-i\omega\tau} d\mathbf{k}' d\omega \quad (12.12)$$

and we define the object  $\tilde{K}_0(\mathbf{k}', \omega)$  [cf. eq. (5.11)] by the relation

$$K_0(\mathbf{R}, \tau) = (2\pi)^{-4} \int \exp(i\mathbf{k}' \cdot \mathbf{R}) e^{-i\omega\tau} \tilde{K}_0(\mathbf{k}', \omega) d\mathbf{k}' d\omega. \quad (12.13)$$

Substituting eqs. (12.12) and (12.13) into eq. (12.11), we then have

$$(2\pi)^{-4} \iint \left[ \left( \hbar\omega - \frac{\hbar^2 k'^2}{2m} \right) \tilde{K}_0(\mathbf{k}', \omega) - 1 \right] \exp\{i(\mathbf{k}' \cdot \mathbf{R} - \omega\tau)\} d\mathbf{k}' d\omega = 0 \quad (12.14)$$

so that

$$\tilde{K}_0(\mathbf{k}', \omega) = \frac{1}{\hbar\omega - \hbar^2 k'^2/2m} \quad (12.15)$$

and therefore we deduce for  $K_0(\mathbf{R}, \tau)$  the integral representation

$$K_0(\mathbf{R}, \tau) = (2\pi)^{-4} \int \frac{\exp\{i(\mathbf{k}' \cdot \mathbf{R} - \omega\tau)\}}{\hbar\omega - \hbar^2 k'^2/2m} d\mathbf{k}' d\omega. \quad (12.16)$$

Let us first consider the integral on the variable  $\omega$ , namely

$$I = \hbar^{-1} \int_{-\infty}^{+\infty} \frac{e^{-i\omega\tau}}{\omega - \omega_0} d\omega \quad (12.17)$$

where  $\omega_0 = \hbar k'^2/2m$ . We see that the integrand has a pole at  $\omega = \omega_0$  so that we must avoid this singularity by choosing an appropriate path in the complex  $\omega$ -plane. As in Section 5.2 the criterion for selecting this path will be that the Green's function leads to a wave function having a physically acceptable behaviour. In Section 5.2 the Green's function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  given by eq. (5.27) was determined by requiring that the stationary scattering wave function  $\psi_{\mathbf{k}_i}^{(+)}$  satisfies the boundary condition (3.27). In the present case the physical requirement will be the concept of *causality*.

To understand how this comes about, let us examine the following expressions

$$I^{(\pm)} = \hbar^{-1} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{e^{-i\omega\tau}}{\omega - \omega_0 \pm i\varepsilon} d\omega \quad (12.18)$$

which are obtained from the quantity  $I$  by shifting the pole of the integrand respectively below and above the real  $\omega$ -axis by a small positive quantity  $\varepsilon \rightarrow 0^+$  (see Fig. 12.1). Since

$$\exp(-i\omega\tau) = \exp(-i\tau \operatorname{Re} \omega) \exp(\tau \operatorname{Im} \omega)$$

it is clear that for negative values of  $\tau$  we should close the integration contour in eq. (12.18) by a large semi-circle  $C_1$  in the *upper* half  $\omega$ -plane ( $\text{Im } \omega > 0$ ).

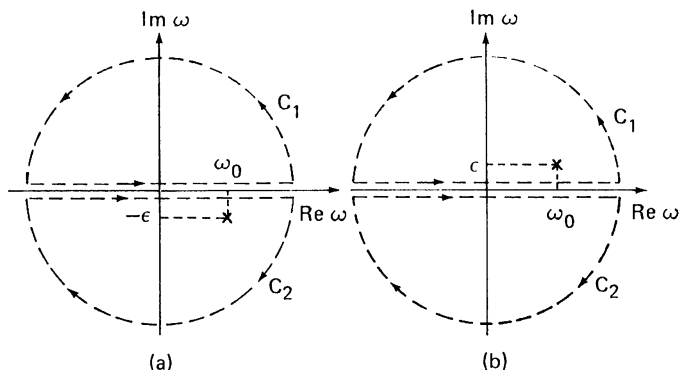


Fig. 12.1. The poles ( $\times$ ) and integration contours  $C_1$  and  $C_2$  which appear in the evaluation (a) of  $I_+$ ; (b) of  $I_-$ . Here  $\omega_0 = \hbar k'^2/2m$ .

Letting the radius of  $C_1$  tend to infinity we therefore obtain immediately

$$I^{(+)}(\tau) = 0, \quad \tau < 0 \quad (12.19)$$

while

$$I^{(-)}(\tau) = \hbar^{-1} 2\pi i \exp(-i\omega_0\tau) \exp(\epsilon\tau), \quad \tau < 0 \quad (12.20)$$

where the limiting process  $\epsilon \rightarrow 0^+$  is implied. Similarly, closing the integration contour in the lower half-plane (contour  $C_2$  of Fig. 12.1) for  $\tau > 0$ , we find that

$$I^{(+)}(\tau) = -\hbar^{-1} 2\pi i \exp(-i\omega_0\tau) \exp(-\epsilon\tau), \quad \tau > 0 \quad (12.21)$$

while

$$I^{(-)}(\tau) = 0, \quad \tau > 0. \quad (12.22)$$

Introducing the step function  $\Theta(\tau)$  such that

$$\Theta(\tau) = \begin{cases} 1, & \tau > 0 \\ 0, & \tau < 0 \end{cases} \quad (12.23)$$

we may rewrite eqs. (12.19)–(12.22) in a more compact way as

$$I^{(+)}(\tau) = -\frac{2\pi i}{\hbar} \exp(-i\omega_0\tau) \exp(-\epsilon\tau) \Theta(\tau) \quad (12.24)$$

and

$$I^{(-)}(\tau) = \frac{2\pi i}{\hbar} \exp(-i\omega_0\tau) \exp(\epsilon\tau) \Theta(-\tau). \quad (12.25)$$

Hence, going back to the integral representation (12.16) we see that the time-dependent Green's function  $K_0^{(+)}(\mathbf{R}, \tau)$  corresponding to  $I^{(+)}$  is given by

$$K_0^{(+)}(\mathbf{R}, \tau) = -(2\pi)^{-3} \frac{i}{\hbar} \exp(-\epsilon\tau) \Theta(\tau) \int \exp(i\mathbf{k}' \cdot \mathbf{R}) \exp\left\{-i \frac{\hbar \mathbf{k}'^2}{2m} \tau\right\} d\mathbf{k}' \quad (12.26)$$



while similarly

$$K_0^{(-)}(\mathbf{R}, \tau) = (2\pi)^{-3} \frac{i}{\hbar} \exp(\varepsilon\tau) \Theta(-\tau) \int \exp(i\mathbf{k}' \cdot \mathbf{R}) \exp\left\{-i \frac{\hbar k'^2}{2m} \tau\right\} d\mathbf{k}'. \quad (12.27)$$

Let us now return to the integral equation (12.9) for the full wave function. Remembering that  $\mathbf{R} = \mathbf{r} - \mathbf{r}'$  and  $\tau = t - t'$  we have

$$\Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \int d\mathbf{r}' \int_{-\infty}^{+\infty} dt' K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \Psi^{(+)}(\mathbf{r}', t'). \quad (12.28)$$

Since the propagator  $K_0^{(+)}$  vanishes for  $t - t' < 0$  we may also write

$$\Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \int d\mathbf{r}' \int_{-\infty}^t dt' K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \Psi^{(+)}(\mathbf{r}', t'). \quad (12.29)$$

On the other hand, the time dependent Green's function  $K_0^{(-)}$  leads to the integral equation

$$\Psi^{(-)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \int d\mathbf{r}' \int_t^{\infty} dt' K_0^{(-)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \Psi^{(-)}(\mathbf{r}', t'). \quad (12.30)$$

Thus the wave function  $\Psi^{(+)}(\mathbf{r}, t)$  is obtained only from values of  $\Psi^{(+)}(\mathbf{r}', t')$  at times  $t' < t$  which are *prior* to  $t$ . On the contrary, the solution  $\Psi^{(-)}(\mathbf{r}, t)$  is constructed from values of  $\Psi^{(-)}(\mathbf{r}', t')$  corresponding to times  $t' > t$ . Hence in order to insure *causal propagation* – so that  $\Psi(\mathbf{r}, t)$  should be determined by values of  $\Psi(\mathbf{r}', t')$  at times  $t' < t$  lying in the *past* – we must adopt the *causal* or *time-retarded* Green's function (or *propagator*)  $K_0^{(+)}$ . The other Green's function  $K_0^{(-)}$  is called the *time-advanced propagator*.

It is a simple matter to obtain from eqs. (12.26) and (12.27) the explicit expressions of the Green's functions  $K_0^{(+)}$  and  $K_0^{(-)}$ . We use Cartesian coordinates such that  $\mathbf{R} \equiv (X, Y, Z)$  and  $\mathbf{k}' \equiv (k'_x, k'_y, k'_z)$ . We then note that

$$\begin{aligned} & \int_{-\infty}^{+\infty} \exp(i\mathbf{k}'_x X) \exp\left\{-i \frac{\hbar k'^2_x}{2m} \tau\right\} dk'_x \\ &= \exp\left\{i \frac{m}{2\hbar\tau} X^2\right\} \int_{-\infty}^{+\infty} \exp\left\{-i \frac{\hbar\tau}{2m} \left(k'_x - \frac{mX}{\hbar\tau}\right)^2\right\} dk'_x \\ &= \exp\left\{i \frac{m}{2\hbar\tau} X^2\right\} \left(\frac{2m}{\hbar\tau}\right)^{1/2} \int_{-\infty}^{+\infty} \exp(-iq_x^2) dq_x \end{aligned} \quad (12.31)$$

where we have set  $q_x = (\hbar\tau/2m)^{1/2}(k'_x - mX/\hbar\tau)$ . The integral appearing on the right-hand side of eq. (12.31) is not strictly convergent, but it can be evaluated by inserting an integration factor  $\exp(-\alpha q_x^2)$  into the integrand (with  $\alpha$  real and positive) and taking the limit  $\alpha \rightarrow 0^+$  at the end of the calculation. Since

$$\int_{-\infty}^{+\infty} \exp\{-(\alpha + i)q_x^2\} dq_x = \left(\frac{\pi}{\alpha + i}\right)^{1/2} \quad (12.32)$$

we then find that

$$\int_{-\infty}^{+\infty} \exp(ik'_x X) \exp\left\{-i\frac{\hbar k_x^2}{2m}\tau\right\} dk'_x = \left(\frac{2\pi m}{i\hbar\tau}\right)^{1/2} \exp\left\{i\frac{m}{2\hbar\tau}X^2\right\}. \quad (12.33)$$

Using similar results for the integration over the variables  $k'_y$  and  $k'_z$  in eq. (12.26) we obtain

$$K_0^{(+)}(\mathbf{R}, \tau) = \frac{(2\pi)^{-3}}{i\hbar} \exp(-\varepsilon\tau) \Theta(\tau) \left(\frac{2\pi m}{i\hbar\tau}\right)^{3/2} \exp\left\{i\frac{m}{2\hbar\tau}R^2\right\}. \quad (12.34)$$

Returning to our original variables  $(\mathbf{r}, t; \mathbf{r}', t')$ , we may also write

$$K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') = \frac{1}{i\hbar} \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \times \exp\{-\varepsilon(t-t')\} \Theta(t-t') \exp\left\{i\frac{m|\mathbf{r}-\mathbf{r}'|^2}{2\hbar(t-t')}\right\} \quad (12.35)$$

or, letting  $\varepsilon \rightarrow 0^+$ , we find that

$$K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') = \frac{1}{i\hbar} \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \Theta(t-t') \exp\left\{i\frac{m|\mathbf{r}-\mathbf{r}'|^2}{2\hbar(t-t')}\right\}. \quad (12.36)$$

Similarly, we obtain for the "advanced" propagator

$$K_0^{(-)}(\mathbf{r}, t; \mathbf{r}', t') = \frac{i}{\hbar} \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \Theta(t'-t) \exp\left\{i\frac{m|\mathbf{r}-\mathbf{r}'|^2}{2\hbar(t-t')}\right\}. \quad (12.37)$$

## 12.2. Time-dependent integral equations

With the causal Green's function determined in the way described above, we may now return to the integral equation (12.29). Thus we have

$$\Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \frac{1}{i\hbar} \int d\mathbf{r}' \int_{-\infty}^t dt' \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \times \exp\left\{i\frac{m|\mathbf{r}-\mathbf{r}'|^2}{2\hbar(t-t')}\right\} V(\mathbf{r}', t') \Psi^{(+)}(\mathbf{r}', t'). \quad (12.38)$$

This is the desired equation which generalizes the results of Chapter 5 and allow us to treat time-dependent interactions. We may also use the expression (12.26) of  $K_0^{(+)}$  to write

$$\Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \frac{1}{i\hbar} (2\pi)^{-3} \int d\mathbf{r}' \int_{-\infty}^t dt' \int d\mathbf{k}' \exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\} \times \exp\left\{-i\frac{\hbar k'^2}{2m}(t-t')\right\} \exp\{-\varepsilon(t-t')\} V(\mathbf{r}', t') \Psi^{(+)}(\mathbf{r}', t'). \quad (12.39)$$

In order to gain some insight into the interpretation of these equations, let us first consider the simple case of scattering by a *time-independent* potential  $V(\mathbf{r})$ . We would then expect to recover the results of Chapter 5. First of all, we may look in this case for stationary solutions of the form

$$\Psi^{(+)}(\mathbf{r}, t) = \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) \exp\left(-\frac{i}{\hbar} E_i t\right) \quad (12.40)$$

where  $\mathbf{k}_i$  is the incident wave vector and  $E_i = \hbar^2 k_i^2 / 2m$  [3]. Furthermore, we have

$$\varphi(\mathbf{r}, t) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_i t\right\} \quad (12.41)$$

so that eq. (12.39) becomes

$$\begin{aligned} \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_i t\right\} &= (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_i t\right\} \\ &+ \frac{1}{i\hbar} (2\pi)^{-3} \int d\mathbf{r}' \int_{-\infty}^t dt' \int d\mathbf{k}' \exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\} \exp\left\{-i\frac{\hbar k'^2}{2m}(t - t')\right\} \\ &\times \exp\{-\varepsilon(t - t')\} V(\mathbf{r}') \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}') \exp\left\{-\frac{i}{\hbar} E_i t'\right\}. \end{aligned} \quad (12.42)$$

Let us perform the integral on the variable  $t'$ . Since

$$\int_{-\infty}^t \exp\left\{i\left(\frac{\hbar k'^2}{2m} - \frac{\hbar k_i^2}{2m} - i\varepsilon\right)t'\right\} dt' = \frac{\exp\{i(\hbar k'^2/2m - \hbar k_i^2/2m - i\varepsilon)t\}}{i(\hbar k'^2/2m - \hbar k_i^2/2m - i\varepsilon)} \quad (12.43)$$

we find from eq. (12.42) after cancelling the common factor  $\exp(-iE_i t/\hbar)$  that

$$\begin{aligned} \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) &= (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \\ &- (2\pi)^{-3} \lim_{\varepsilon \rightarrow 0^+} \int d\mathbf{r}' \int d\mathbf{k}' \frac{\exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\}}{k'^2 - k_i^2 - i\varepsilon} U(\mathbf{r}') \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}') \end{aligned} \quad (12.44)$$

where  $U(\mathbf{r}) = 2mV(\mathbf{r})/\hbar^2$  is the reduced potential. We see that eq. (12.44) is precisely the *Lippmann–Schwinger equation* (5.33), namely

$$\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) + \int G_0^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}') d\mathbf{r}' \quad (12.45)$$

where the time-independent Green's function  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  is given by eqs. (5.27) or (5.30) with  $k = k_i$ .

Let us now analyze the equations (12.38) or (12.39) from a more general point of view. Instead of replacing  $V(\mathbf{r}, t)$  by a purely time-independent potential  $V(\mathbf{r})$ , as we did above, we may imagine that the interaction is “switched on” at a certain instant  $t = 0$  and “switched off” at the time  $t$  while remaining time-independent between the two times 0 and  $t$ . Thus we

may write in this case eq. (12.38) as

$$\begin{aligned} \Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \frac{1}{i\hbar} \int d\mathbf{r}' \int_0^t dt' \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \\ \times \exp\left\{ i \frac{m|\mathbf{r} - \mathbf{r}'|^2}{2\hbar(t-t')} \right\} V(\mathbf{r}') \Psi^{(+)}(\mathbf{r}', t'). \end{aligned} \quad (12.46)$$

We shall return to this equation in the next section. Another possibility would be to “switch on” the interaction in an adiabatic way by writing

$$V(\mathbf{r}, t) = V(\mathbf{r}) \exp(-\varepsilon|t|) \quad (12.47)$$

where  $\varepsilon$  is again a very small quantity, real and positive. In this way the interaction is “switched off” in the very remote past and slowly “turned on” as time proceeds. Insertion of the interaction (12.47) into eq. (12.38) then yields again the Lippmann–Schwinger equation (12.44). Thus the “ $i\varepsilon$  prescription” may also be considered as arising from the condition that in the very remote past there is no interaction, so that the state vector then describes free particles.

Before we conclude this section let us remark that a compact solution of the integral equation (12.28) may be formally written down by using a method completely similar to the one we used in Section 5.4. Thus, writing

$$\Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + X^{(+)}(\mathbf{r}, t) \quad (12.48)$$

and substituting into eq. (12.8) we find by using eq. (12.6) that

$$\left[ i\hbar \frac{\partial}{\partial t} - H_0 - V(\mathbf{r}, t) \right] X^{(+)}(\mathbf{r}, t) = V(\mathbf{r}, t) \varphi^{(+)}(\mathbf{r}, t). \quad (12.49)$$

If we know the total time-dependent causal Green's function  $K^{(+)}(\mathbf{r}, t; \mathbf{r}', t')$  satisfying the equation

$$\left[ i\hbar \frac{\partial}{\partial t} - H_0 - V(\mathbf{r}, t) \right] K^{(+)}(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \quad (12.50)$$

then we may obtain explicitly the wave function  $\Psi^{(+)}(\mathbf{r}, t)$  as

$$\Psi^{(+)}(\mathbf{r}, t) = \varphi(\mathbf{r}, t) + \int d\mathbf{r}' \int dt' K^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \varphi(\mathbf{r}', t'). \quad (12.51)$$

Moreover, since eq. (12.50) may be rewritten as

$$\begin{aligned} \left[ i\hbar \frac{\partial}{\partial t} - H_0 \right] K^{(+)}(\mathbf{r}, t; \mathbf{r}', t') \\ = \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') + V(\mathbf{r}, t) K^{(+)}(\mathbf{r}, t; \mathbf{r}', t') \end{aligned} \quad (12.52)$$

we also find with the help of eq. (12.10) that the total causal Green's function satisfies the integral equation

$$\begin{aligned} K^{(+)}(\mathbf{r}, t; \mathbf{r}', t') = K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') \\ + \int d\mathbf{r}'' \int dt'' K_0^{(+)}(\mathbf{r}, t; \mathbf{r}'', t'') V(\mathbf{r}'', t'') K^{(+)}(\mathbf{r}'', t''; \mathbf{r}', t'). \end{aligned} \quad (12.53)$$

Similar results obviously hold for the corresponding “advanced” total propagator  $K^{(-)}(\mathbf{r}, t; \mathbf{r}', t')$ .

### 12.3. Time-dependent perturbation theory

In this section we want to obtain the time-dependent wave function  $\Psi^{(+)}(\mathbf{r}, t)$  by using perturbation theory. We shall first study an iterative method analogous to the *Born series* of Chapter 8 and then discuss the *method of variation of the constants*.

#### 12.3.1. The Born series for the time-dependent wave function

Let us attempt to solve the integral equation (12.28) by iteration, starting with the unperturbed solution  $\varphi(\mathbf{r}, t)$  given by eq. (12.41). We obtain in this way the *Born sequence* of functions

$$\begin{aligned}\Psi_0(\mathbf{r}, t) &= \varphi(\mathbf{r}, t), \\ \Psi_1(\mathbf{r}, t) &= \varphi(\mathbf{r}, t) + \int K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \varphi(\mathbf{r}', t') d\mathbf{r}' dt' \\ \Psi_2(\mathbf{r}, t) &= \varphi(\mathbf{r}, t) + \int K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \Psi_1(\mathbf{r}', t') d\mathbf{r}' dt' \\ &\vdots \\ \Psi_n(\mathbf{r}, t) &= \varphi(\mathbf{r}, t) + \int K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t') \Psi_{n-1}(\mathbf{r}', t') d\mathbf{r}' dt' \quad (12.54)\end{aligned}$$

The corresponding *Born series* for the function  $\Psi^{(+)}(\mathbf{r}, t)$  is therefore given by

$$\Psi^{(+)}(\mathbf{r}, t) = \sum_{n=0}^{\infty} \chi_n(\mathbf{r}, t) \quad (12.55)$$

with

$$\begin{aligned}\chi_0(\mathbf{r}, t) &= \varphi(\mathbf{r}, t) \\ \chi_n(\mathbf{r}, t) &= \int \mathcal{K}_n(\mathbf{r}, t; \mathbf{r}', t') \varphi(\mathbf{r}', t') d\mathbf{r}' dt', \quad (12.56)\end{aligned}$$

$$\mathcal{K}_n(\mathbf{r}, t; \mathbf{r}', t') = \int \mathcal{K}_1(\mathbf{r}, t; \mathbf{r}'', t'') \mathcal{K}_{n-1}(\mathbf{r}'', t''; \mathbf{r}', t') d\mathbf{r}'' dt'', \quad n > 1 \quad (12.57)$$

and

$$\mathcal{K}_1(\mathbf{r}, t; \mathbf{r}', t') = K_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') V(\mathbf{r}', t'). \quad (12.58)$$

We see that the Born series (12.55) is a perturbation expansion in powers of the interaction.

Let us examine more closely the first order wave function  $\Psi_1(\mathbf{r}, t)$  [4]. Using eqs. (12.36) and (12.41), we find that

$$\begin{aligned}\Psi_1(\mathbf{r}, t) &= \Phi_{\mathbf{k}_i}(\mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_i t\right\} + \frac{1}{i\hbar} \int d\mathbf{r}' \int_{-\infty}^t dt' \left[ \frac{m}{2\pi i \hbar (t - t')} \right]^{3/2} \\ &\quad \times \exp\left\{ \frac{im|\mathbf{r} - \mathbf{r}'|^2}{2\hbar(t - t')} \right\} V(\mathbf{r}', t') \Phi_{\mathbf{k}_i}(\mathbf{r}') \exp\left\{-\frac{i}{\hbar} E_i t'\right\} \quad (12.59)\end{aligned}$$

where  $\Phi_{k_i}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r})$ . In order to simplify the discussion we shall consider the simple case of a perturbation  $V$  which is time-independent, except that it is "switched on" at the time  $t = 0$  and "switched off" at the time  $t$ . We then have

$$\Psi_1(\mathbf{r}, t) = \Phi_{k_i}(\mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_i t\right\} + \frac{1}{i\hbar} \int d\mathbf{r}' \int_0^t dt' \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \times \exp\left\{ \frac{im|\mathbf{r} - \mathbf{r}'|^2}{2\hbar(t-t')} \right\} V(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') \exp\left\{-\frac{i}{\hbar} E_i t'\right\}. \quad (12.60)$$

Since we are ultimately interested in evaluating scattering cross sections and therefore *transition probabilities*, we want to obtain the probability amplitude  $a_{fi}^{(1)}$  of finding the final state

$$\varphi_f(\mathbf{r}, t) = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_f t\right\} = \Phi_{k_f}(\mathbf{r}) \exp\left\{-\frac{i}{\hbar} E_f t\right\} \quad (12.61)$$

in the initial state  $\Psi_1(\mathbf{r}, t)$ . Using the more explicit notation  $\Psi_i^{(1)}(\mathbf{r}, t) \equiv \Psi_1(\mathbf{r}, t)$ , we have when  $f \neq i$

$$a_{fi}^{(1)}(t) = \langle \varphi_f | \Psi_i^{(1)} \rangle = \frac{1}{i\hbar} \int d\mathbf{r} \int d\mathbf{r}' \int_0^t dt' \left[ \frac{m}{2\pi i\hbar(t-t')} \right]^{3/2} \times \exp\left\{ \frac{im|\mathbf{r} - \mathbf{r}'|^2}{2\hbar(t-t')} \right\} \Phi_{k_f}^*(\mathbf{r}) V(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') \exp\left\{\frac{i}{\hbar} E_f t\right\} \exp\left\{-\frac{i}{\hbar} E_i t'\right\}. \quad (12.62)$$

Most of the contribution to the  $t'$ -integral comes from the region where  $t' \simeq t$ . Thus, replacing  $t$  by  $t'$  in  $\exp(iE_f t/\hbar)$  and setting  $u = t - t'$ , we find that

$$a_{fi}^{(1)}(t) = \frac{1}{i\hbar} \left( \frac{m}{2\pi i\hbar} \right)^{3/2} \exp(i\omega_{fi} t) \int d\mathbf{r} \int d\mathbf{r}' \int_0^t du u^{-3/2} \times \exp\left\{ \frac{im|\mathbf{r} - \mathbf{r}'|^2}{2\hbar u} \right\} \Phi_{k_f}^*(\mathbf{r}) V(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') \exp(-i\omega_{fi} u) \quad (12.63)$$

where the quantity  $\omega_{fi}$  is given by

$$\omega_{fi} = (E_f - E_i)/\hbar. \quad (12.64)$$

Introducing the new variable

$$z = 2i\hbar u/m \quad (12.65)$$

we may write eq. (12.63) as

$$a_{fi}^{(1)}(t) = \frac{m}{2\hbar^2} \pi^{-3/2} \exp(i\omega_{fi} t) \int d\mathbf{r} \int d\mathbf{r}' \int_{2i\hbar t/m}^0 dz z^{-3/2} \times \exp\left\{ -\frac{|\mathbf{r} - \mathbf{r}'|^2}{z} \right\} \Phi_{k_f}^*(\mathbf{r}) V(\mathbf{r}') \Phi_{k_i}(\mathbf{r}') \exp\left\{ -\omega_{fi} \frac{m}{2\hbar} z \right\} \quad (12.66)$$

and the bulk of this integral arises from the neighbourhood of  $z = 0$ . Now, since

$$\lim_{z \rightarrow 0} \pi^{-3/2} \frac{\exp(-|\mathbf{r} - \mathbf{r}'|^2/z)}{z^{3/2}} = \delta(\mathbf{r} - \mathbf{r}') \quad (12.67)$$

we see that

$$a_{fi}^{(1)}(t) = \frac{m}{2\hbar^2} \exp(i\omega_{fi}t) \langle f|V|i \rangle \int_{2i\hbar t/m}^0 \exp\left\{-\omega_{fi} \frac{m}{2\hbar} z\right\} dz \quad (12.68)$$

where we have defined

$$\langle f|V|i \rangle \equiv \langle \mathbf{k}_f|V|\mathbf{k}_i \rangle = \int \Phi_{\mathbf{k}_f}^*(\mathbf{r}) V(\mathbf{r}) \Phi_{\mathbf{k}_i}(\mathbf{r}) d\mathbf{r}. \quad (12.69)$$

Performing the  $z$ -integration in eq. (12.68), we then obtain

$$a_{fi}^{(1)}(t) = -\frac{\langle f|V|i \rangle}{\hbar\omega_{fi}} \{\exp(i\omega_{fi}t) - 1\} \quad (12.70)$$

which is our final result for the *probability amplitude* corresponding to the transition  $i \rightarrow f$ , calculated to *first order* of perturbation theory. Higher order approximations are obtained in a similar way from the wave functions  $\Psi_2, \dots, \Psi_n$  of eq. (12.54).

### 12.3.2. The method of variation of the constants

Before we analyze in more detail the probability amplitude  $a_{fi}^{(1)}$  and the corresponding *transition probability*  $|a_{fi}^{(1)}|^2$ , we shall describe an alternative method of formulating time-dependent perturbation theory, which is known as the *method of variation of the constants* [5]. Since this approach is discussed in any textbook on quantum mechanics [see e.g. 6–8] we shall only give here an outline of the method.

Let us start from the time-dependent Schrödinger equation (12.1) and write the total Hamiltonian  $H$  as

$$H = H_0 + H_1 \quad (12.71)$$

where the “unperturbed” Hamiltonian  $H_0$  is time-independent and  $H_1$  is a time-dependent perturbation. We shall first give a brief summary of the method for a general Hamiltonian  $H$  such that a separation of the type (12.71) is meaningful; the application to the particular Hamiltonian (12.2) will be made subsequently.

We assume that the eigenvalues  $E_n$  and the stationary normalized eigenfunctions  $\Phi_n$  of the unperturbed Hamiltonian  $H_0$  are known. Thus

$$H_0 \Phi_n = E_n \Phi_n \quad (12.72)$$

so that the general solution of the equation

$$H_0 \Psi_0 = i\hbar \frac{\partial}{\partial t} \Psi_0 \quad (12.73)$$

is given by

$$\Psi_0 = \sum_n c_n \Phi_n \exp\left(-\frac{i}{\hbar} E_n t\right) \quad (12.74)$$

where the coefficients  $c_n$  are *constants* and the symbol  $\sum_n$  implies a summation over the discrete set together with an integration over the continuous set of eigenfunctions. Returning to the original Schrödinger equation (12.1), and by analogy with eq. (12.74) we write the unknown wave function  $\Psi$  as

$$\Psi = \sum_n a_n(t) \Phi_n \exp\left(-\frac{i}{\hbar} E_n t\right) \quad (12.75)$$

where the unknown coefficients  $a_n(t)$  must clearly depend on the time. Substitution of eq. (12.75) into eq. (12.1) yields

$$\begin{aligned} \sum_n a_n (H_0 + H_1) \Phi_n \exp\left(-\frac{i}{\hbar} E_n t\right) &= i\hbar \sum_n \dot{a}_n \Phi_n \exp\left(-\frac{i}{\hbar} E_n t\right) \\ &\quad + \sum_n a_n E_n \Phi_n \exp\left(-\frac{i}{\hbar} E_n t\right) \end{aligned} \quad (12.76)$$

where we have used eq. (12.71) and the dot denotes a derivative with respect to the time. Using eq. (12.72) and taking the inner product on the left with  $\Phi_k$ , we find that

$$\dot{a}_k(t) = (i\hbar)^{-1} \sum_n a_n(t) \langle k | H_1 | n \rangle \exp(i\omega_{kn}t), \quad k = 1, 2, \dots \quad (12.77)$$

where  $\omega_{kn} = (E_k - E_n)/\hbar$  [see eq. (12.64)] while

$$\langle k | H_1 | n \rangle \equiv \langle \Phi_k | H_1 | \Phi_n \rangle. \quad (12.78)$$

The system of coupled differential equations (12.77) is strictly equivalent to the original Schrödinger equation (12.1), and no approximation has been made so far. At this point, however, we elect to solve the system (12.77) by using perturbation theory. To this end, we write

$$H = H_0 + \lambda H_1 \quad (12.79)$$

and expand the coefficients  $a_n$  in powers of the parameter  $\lambda$  [9] as

$$a_n = a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)} + \dots \quad (12.80)$$

Substituting the expansion (12.80) into the system (12.77), replacing in  $H_1$  by  $\lambda H_1$  and equating the coefficients of equal powers of  $\lambda$ , we find that

$$\dot{a}_k^{(0)} = 0 \quad (12.81a)$$

$$\dot{a}_k^{(1)} = (i\hbar)^{-1} \sum_n \langle k | H_1 | n \rangle \exp(i\omega_{kn}t) a_n^{(0)} \quad (12.81b)$$

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$$\dot{a}_k^{(s+1)} = (i\hbar)^{-1} \sum_n \langle k | H_1 | n \rangle \exp(i\omega_{kn}t) a_n^{(s)}, \quad s = 0, 1, 2, \dots \quad (12.81c)$$



We see that the original system (12.77) has now been decoupled in such a way that eqs. (12.81) may – in principle – be integrated successively to any given order. The first equation (12.81a) simply states that the coefficients  $a_k^{(0)}$  are time-independent. These are clearly the *initial conditions* of the problem. Indeed, before the perturbation is applied, the quantities  $a_k^{(0)}$  are identical to the coefficients  $c_k$  of a particular solution of the unperturbed problem. Hence  $|a_k^{(0)}|^2$  gives the probability of finding the system in the stationary state  $|\Phi_k\rangle \equiv |k\rangle$  before the perturbation is applied. Similarly, the quantity  $|a_k(t)|^2$  yields the probability of finding the system in the state  $|k\rangle$  at the time  $t$ .

Let us assume that the system which we consider is initially in a well defined stationary state  $|\Phi_i\rangle \equiv |i\rangle$ . Since we have essentially an infinite amount of time at our disposal to “prepare” this initial state, the above statement is not in contradiction with the uncertainty relation  $\Delta E \Delta t \geq \hbar$ . We then have

$$a_k^{(0)} = \begin{cases} \delta_{ki} & \text{for discrete states,} \\ \delta(k-i) & \text{for continuous states.} \end{cases} \quad (12.82)$$

From eqs. (12.81b) and (12.82) we deduce that

$$a_{ki}^{(1)}(t) = (i\hbar)^{-1} \int_{-\infty}^t \langle k|H_1|i\rangle \exp(i\omega_{ki}t') dt' \quad (12.83)$$

where we have chosen the integration constant in such a way that one has initially  $a_{ki}^{(1)}(-\infty) = 0$ . We have also written explicitly  $a_{ki}^{(1)}$  with a subscript  $i$  to emphasize that it arises from the initial state  $|i\rangle$ . Thus the quantity

$$W_{ki}^{(1)}(t) = |a_{ki}^{(1)}(t)|^2 \quad (12.84)$$

yields – to first order in the perturbation calculation – the transition probability from the initial state  $|i\rangle$  to a particular state  $|k\rangle$ .

The relation (12.83) becomes particularly simple if the perturbation  $H_1$  is “turned on” at the time  $t_0 = 0$  and “turned off” at the time  $t$ , while remaining time-independent during the time interval  $(0, t)$ . We then have

$$a_{ki}^{(1)}(t) = - \frac{\langle k|H_1|i\rangle}{\hbar\omega_{ki}} \{\exp(i\omega_{ki}t) - 1\}. \quad (12.85)$$

Let us now return to time-dependent potential scattering, for which  $H_0 = -\hbar^2\nabla_r^2/2m$ ,  $H_1 = V(r, t)$  and assume that  $V(r, t)$  is “switched on” at  $t = 0$ , “switched off” at the time  $t$  and is equal to  $V(r)$  during the interval  $(0, t)$ . We see that in this case eq. (12.85) is identical to the result (12.70) which we found from the time-dependent integral equation (12.28) by means of first order perturbation theory.

### 12.4. Transition probabilities and cross sections

Having obtained to first order of perturbation theory the probability amplitude  $a_{ki}^{(1)}$  for the transition  $i \rightarrow k$  induced by the perturbation  $V(\mathbf{r}, t)$  acting between the times 0 and  $t$ , we may now write the corresponding first order transition probability as

$$W_{ki}^{(1)}(t) = |a_{ki}^{(1)}(t)|^2 = |\langle k|V|i\rangle|^2 \frac{4 \sin^2 \frac{1}{2}\omega_{ki}t}{\hbar^2 \omega_{ki}^2} \quad (12.86)$$

or

$$W_{ki}^{(1)}(t) = \frac{4}{\hbar^2} |\langle k|V|i\rangle|^2 f(t, \omega_{ki}) \quad (12.87)$$

where we have set

$$f(t, \omega_{ki}) = (\sin^2 \frac{1}{2}\omega_{ki}t)/\omega_{ki}^2. \quad (12.88)$$

The quantity  $f(t, \omega_{ki})$  is displayed in Fig. 12.2 as a function of  $\omega_{ki}$  (for fixed  $t$ ). We note that  $f(t, \omega_{ki})$  exhibits a very pronounced peak around the value  $\omega_{ki} = 0$ ; the height of this peak is proportional to  $t^2$ , while its width is given by  $2\pi/t$ . A simple calculation using the residue theorem shows that

$$\int_{-\infty}^{+\infty} f(t, \omega_{ki}) d\omega_{ki} = \frac{1}{2}\pi t \quad (12.89)$$

so that the area under the curve in Fig. 12.2 is proportional to  $t$ . Moreover, one also has [see e.g. 7]

$$f(t, \omega_{ki}) \underset{t \rightarrow \infty}{\sim} \frac{1}{2}\pi t \delta(\omega_{ki}). \quad (12.90)$$

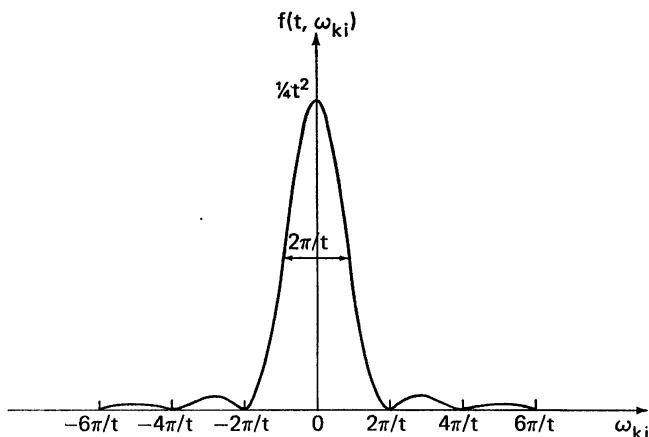


Fig. 12.2. The quantity  $f(t, \omega_{ki})$  as a function of  $\omega_{ki}$ , for fixed  $t$ .

Let us now consider again eq. (12.87). The sharp peak of the factor  $f(t, \omega_{ki})$  around the value  $\omega_{ki} = 0$  favors very strongly the transition towards those final states  $k$  for which the quantity  $\omega_{ki}$  does not deviate from zero by an amount larger than  $\delta\omega_{ki} \simeq 2\pi/t$ . Thus the transitions occur mainly

towards those final states whose energies  $E_k$  do not differ from the initial energy  $E_i$  by more than

$$\delta E \simeq 2\pi\hbar/t. \quad (12.91)$$

Hence the transitions conserve approximately the energy, the spread in energy being given by  $2\pi\hbar/t$ .

It is interesting to relate this result with the time-energy uncertainty relation  $\Delta E \Delta t \gtrsim \hbar$ . Since the perturbation gives a way of measuring the energy of the system by inducing transitions  $i \rightarrow k$ , and because the time of action of the perturbation is  $t$ , the uncertainty related to this measurement should be approximately  $\hbar/t$ , in qualitative agreement with the result (12.91).

It is apparent from the foregoing discussion that for processes which occur in the *continuum* part of the spectrum, we must consider transitions to one or several groups of final states  $|k\rangle$  whose energy  $E_k$  lies within a given interval  $(E_f - \eta, E_f + \eta)$  centered about the value  $E_f$ . Let us first consider the simple case of *one* group of states  $|k\rangle$ . We denote by  $\rho_k(E_k)$  a *density of levels* such that  $\rho_k(E_k) dE_k$  is the number of states  $|k\rangle$  within the energy interval  $(E_k, E_k + dE_k)$ . The first order transition probability from the initial state  $|i\rangle$  to the group of final state  $|k\rangle$  is then given by

$$W_{fi}^{(1)}(t) = \int_{E_f - \eta}^{E_f + \eta} W_{ki}^{(1)}(t) \rho_k(E_k) dE_k \quad (12.92)$$

where  $W_{ki}^{(1)}$  is given by eq. (12.87). Assuming that  $\eta$  is small enough so that  $\langle k|V|i\rangle$  and  $\rho_k$  are nearly constant within the integration range, we have

$$W_{fi}^{(1)}(t) = \frac{4}{\hbar} |\langle f|V|i\rangle|^2 \rho_f(E_f) \int_{\omega_f - \eta'}^{\omega_f + \eta'} f(t, \omega_{ki}) d\omega_{ki} \quad (12.93)$$

where we have changed the integration variable to  $\omega_{ki} = (E_k - E_i)/\hbar$  and the state  $|f\rangle$  belonging to the group has the energy  $E_f$ . We have also set  $\eta' = \eta/\hbar$  and we shall assume that  $\eta' \gg 2\pi/t$ .

It is clear from the above discussion that the overwhelming part of the integral on the right-hand side of eq. (12.93) arises from those transitions  $i \rightarrow k$  which *conserve the energy* (within  $\delta E \simeq 2\pi\hbar/t$ ). Indeed, in this case  $\omega_{fi} \simeq 0$  so that the peak of the function  $f(t, \omega_{ki})$  [occurring at  $\omega_{ki} = 0$ ] lies within the integration range. Then since  $\eta' \gg 2\pi/t$  we may write

$$\int_{\omega_f - \eta'}^{\omega_f + \eta'} f(t, \omega_{ki}) d\omega_{ki} \simeq \int_{-\infty}^{+\infty} f(t, \omega_{ki}) d\omega_{ki} = \frac{1}{2}\pi t \quad (12.94)$$

and therefore

$$W_{fi}^{(1)}(t) = \frac{2\pi}{\hbar} |\langle f|V|i\rangle|^2 \rho_f(E) t \quad (12.95)$$

with  $E = E_i = E_f$ .

We are now in a position to evaluate the physically interesting quantity, namely the (first order) *transition probability per unit time*. It is given by

$$w_{fi}^{(1)} = \frac{d}{dt} W_{fi}^{(1)}(t) \quad (12.96)$$

or

$$w_{fi}^{(1)} = \frac{2\pi}{\hbar} |\langle f|V|i\rangle|^2 \rho_f(E). \quad (12.97)$$

This formula, first obtained by Dirac [5], has played such an important role in time-dependent problems that Fermi called it the Golden Rule [10]. We may easily generalize it to the case where there are several groups of final states  $|f\rangle$  having an energy in the neighbourhood of  $E_i$ , but for which the quantity  $\langle f|V|i\rangle$  and (or) the density of levels  $\rho_f$  may vary from one group to the other. In this case eq. (12.97) gives the transition probability per unit time for a given group, and the total value of  $w_{fi}^{(1)}$  is

$$w_{fi}^{(1)}(\text{total}) = \frac{2\pi}{\hbar} \sum_{f'} |\langle f'|V|i\rangle|^2 \rho_{f'}(E) \quad (12.98)$$

where the summation runs over the groups considered.

Let us illustrate these considerations by returning to the analysis of our scattering problem. In this case there are many different final free (plane wave) states  $|k_f\rangle$  corresponding to the energy  $E = \hbar^2 k^2/2m$ , but to different directions of the wave vector  $k_f$ . Let us denote by  $\rho_f(E) d\Omega dE$  the number of states whose wave vector  $k_f$  lies within the solid angle  $d\Omega$  and whose energy is in the interval  $(E, E + dE)$ . Then, because of our “normalization” of plane waves [see eqs. (5.6)–(5.8)] we have

$$\rho_f(E) d\Omega dE = dk_f = k^2 dk d\Omega \quad (12.99)$$

so that the *density of final states*  $\rho_f(E)$  (i.e. the density of levels within the particular *subgroup* of final states whose wave vectors  $k_f$  lie within  $d\Omega$ ) is given by

$$\rho_f(E) = k^2 dk/dE \quad (12.100)$$

or

$$\rho_f(E) = mk/\hbar^2. \quad (12.101)$$

It is worth emphasizing that  $\rho_f(E)$  depends on the normalization [11] adopted for the free states  $|k_f\rangle$ .

The first order transition probability per unit time corresponding to particles scattered within an element of solid angle  $d\Omega$  is then given by

$$dw_{fi}^{(1)} = \frac{2\pi}{\hbar} |\langle f|V|i\rangle|^2 \rho_f(E) d\Omega. \quad (12.102)$$

It is now a simple matter to obtain (to first order) the differential scattering cross section corresponding to the transition  $k_i \rightarrow k_f$ . Applying the definition

of Section 1.3, we first calculate the incident flux  $\Phi_A$  corresponding to the plane wave  $\langle \mathbf{r} | \mathbf{k}_i \rangle = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r})$ . That is,

$$\Phi_A = (2\pi)^{-3} \frac{\hbar k}{m} = (2\pi)^{-3} v \quad (12.103)$$

where  $v = |\mathbf{v}_i|$  is the magnitude of the incident velocity. Then, dividing the quantity  $d\omega_{fi}^{(1)}$  by  $\Phi_A$  we find that

$$d\sigma^{(1)} = \frac{(2\pi)^4}{\hbar v} |\langle f | V | i \rangle|^2 \rho_f(E) d\Omega. \quad (12.104)$$

Hence

$$\frac{d\sigma^{(1)}}{d\Omega} = \frac{(2\pi)^4}{\hbar v} |\langle f | V | i \rangle|^2 \rho_f(E) \quad (12.105)$$

or, using eqs. (12.69) and (12.101), we have

$$\frac{d\sigma^{(1)}}{d\Omega} = (16\pi^2)^{-1} \left| \int \exp(i\mathbf{A} \cdot \mathbf{r}) U(\mathbf{r}) d\mathbf{r} \right|^2 \quad (12.106)$$

with  $\mathbf{A} = \mathbf{k}_i - \mathbf{k}_f$  and  $U(\mathbf{r}) = 2mV(\mathbf{r})/\hbar^2$ . The result (12.106) is precisely the first Born differential cross section [see eqs. (8.30)–(8.31)]. We have therefore rederived to first order – and within the conditions discussed above – the results of the time-independent theory.

We shall not attempt here to obtain transition probabilities beyond the first order of perturbation theory. This problem will be discussed in Chapter 15 in a more general context.

## References and notes

- [1] The time-dependent Green's function technique which we use in this section is quite general and may be applied to a variety of equations of first order in the time derivative. See for example BYRON JR., F. W. and R. W. FULLER (1970), *Mathematics of Classical and Quantum Physics* (Addison-Wesley, Reading, Mass.) Vol. II, Chapter 7, Section 7.7.
- [2] Propagators play a central role in Feynman's formulation of quantum mechanics. A detailed discussion may be found in FEYNMAN, R. P. and A. R. HIBBS (1965), *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York).
- [3] In what follows we shall write explicitly  $E_i = \hbar^2 k_i^2/2m$  and  $E_f = \hbar^2 k_f^2/2m$ . This notation is convenient in view of later developments.
- [4] We follow here the treatment of ROMAN, P. (1965), *Advanced Quantum Theory* (Addison-Wesley, Reading, Mass.) Chapter 3.
- [5] DIRAC, P. A. M. (1926), Proc. Roy. Soc. **A112**, 661; (1927), **A114**, 273.
- [6] SCHIFF, L. I. (1955), *Quantum Mechanics* (McGraw-Hill, New York) Chapter 8.
- [7] MESSIAH, A. (1966), *Quantum Mechanics* (Wiley, New York) Vol. II, Chapter 17.
- [8] MERZBACHER, E. (1970), *Quantum Mechanics* (Wiley, New York) Chapter 18.

- [9] The purpose of introducing the parameter  $\lambda$  is simply to identify the various orders in the perturbation;  $\lambda$  is then set equal to one when this identification has been made.
- [10] It is clear that the Golden Rule holds equally well for a system described by the general Hamiltonian  $H = H_0 + H_1$ , where  $H_0$  is time-independent and the perturbation  $H_1$  is also independent of  $t$  except that it is switched on at one time and off later on. In this case one has  $w_{fi}^{(1)} = (2\pi/\hbar) \langle f | H_1 | i \rangle^2 \rho_f(E)$ .
- [11] This may be seen as follows. Let us assume that the free states  $|k\rangle$  are normalized in such a way that

$$\langle k' | k \rangle = \delta(k - k')/N(k)$$

and

$$\int dk |k\rangle N(k) \langle k| = 1$$

where  $N(k)$  is a real, positive function. The number of states in the interval  $(k, k + dk)$  is then given by  $N(k) dk$ . Hence the number of states  $|k\rangle$  whose wave vector lies in the solid angle  $(\Omega, \Omega + d\Omega)$  and whose energy  $E = \hbar^2 k^2/2m$  is in the band  $(E, E + dE)$  is given by

$$\rho(E) d\Omega dE = N(k) dk = N(k) k^2 dk d\Omega$$

so that

$$\rho(E) = N(k) k^2 dk/dE.$$

The "normalization" chosen in the text is such that  $N(k) = 1$ .

# Problems to Part II

1. Obtain the phase shifts  $\delta_l$  produced by a repulsive potential of the form  $V(r) = A/r^2$  ( $A > 0$ ). Discuss the angular distribution. Is the total cross section finite? Explain. [Note: For given  $v$  and large  $x$  one has  $j_v(x) \sim \sin(x - \frac{1}{2}v\pi)/x$ .]
2. Consider now an attractive potential given by  $V(r) = A/r^2$  ( $A < 0$ ). How must the treatment of Problem 1 be modified? Show that there is only a restricted range of values for  $A$  such that the radial Schrödinger equation (4.17) has acceptable solutions.
3. Assume that in a given elastic scattering experiment between two particles without structure the center of mass differential cross section  $d\sigma/d\Omega$  may be represented by an expression of the type
 
$$d\sigma/d\Omega = A + BP_1(\cos \theta) + CP_2(\cos \theta).$$
 Express the coefficients  $A$ ,  $B$  and  $C$  in terms of the (real) phase shifts  $\delta_l$ .
4. In a certain nuclear elastic scattering experiment carried out at low energies ( $k = 3 \times 10^{12} \text{ cm}^{-1}$ ), differential cross sections are measured for 10 values of  $\cos \theta$ , where  $\theta$  is the scattering angle in the center of mass system. The results are the following:

$\cos \theta$	$d\sigma/d\Omega$ (in mb/sr)
0.9	8.0
0.7	7.2
0.5	6.9
0.3	6.2
0.1	5.6
-0.1	5.0
-0.3	4.4
-0.5	4.0
-0.7	3.2
-0.9	2.5

Each measurement of  $d\sigma/d\Omega$  is estimated to have a  $\pm 5\%$  error.

a) Determine approximately the  $l = 0$  and  $l = 1$  (real) phase shifts, neglecting phase shifts with  $l \geq 2$ . Show that the resultant error in  $\delta_1$  is greater than the error in  $\delta_0$ .

b) Assume that it is known that the two particles cannot form a bound state. How will this information be useful in making the analysis of (a) more precise?

c) Estimate to what extent the neglect of the partial waves higher than  $l = 1$  is justified by the data.

5. Consider the low-energy scattering produced by a real potential of finite range  $a$ . Assume that the scattering is non-resonant and that the phase shifts with  $l \geq 2$  may be neglected. Show that the influence of the p-wave phase shift  $\delta_1$  is much stronger on the angular distribution than on the total cross section. In particular, analyze the contribution of the s- and p-waves to the differential and total cross sections when  $ka = 0.3$ ,  $\delta_0 = 25^\circ$  and  $\delta_1 = 2^\circ$ .
6. Using the first three partial waves ( $l = 0, 1, 2$ ), study the low-energy scattering by an attractive square well potential of (reduced) strength  $U_0$  and range  $a$ . In particular, plot the phase shifts, the partial wave cross sections and the total cross section as a function of  $ka$  when  $0 \leq ka \leq 2$  and (i)  $U_0 a^2 = 1$ , (ii)  $U_0 a^2 = 10$ .
7. Determine the total cross section for low-energy (s-wave) scattering by a potential barrier such that

$$U(r) = \begin{cases} U_0 (> 0), & r < a \\ 0, & r > a. \end{cases}$$

Obtain the "hard sphere" low-energy result  $\sigma_{\text{tot}} = 4\pi a^2$  as a limiting case.

8. Using the first four partial waves, obtain the differential and total cross sections for the scattering by a hard sphere when the reduced de Broglie wavelength  $\lambda = k^{-1}$  of the incident particle is equal to the radius  $a$  of the sphere. Discuss the accuracy of your results.
9. Show that the first Born approximation (8.74) for  $\tan \delta_l$  leads to the first Born scattering amplitude (8.35) if  $\delta_l \ll 1$  for all values of  $l$ . [Hint: Use the fact that

$$j_0(\Delta r) = \sum_{l=0}^{\infty} (2l+1) j_l^2(kr) P_l(\cos \theta).]$$

10. Consider the partial wave expansion (4.64) of the scattering amplitude, namely

$$f(k, \theta) = \sum_{l=0}^{\infty} (2l+1) a_l(k) P_l(\cos \theta).$$



- a) Write a general expression for  $a_l(k)$  in terms of  $f(k, \theta)$ .
- b) Assume that we are dealing with a Yukawa potential  $U(r) = U_0 e^{-ar}/r$ . Using the Born approximation to  $f(k, \theta)$ , find  $a_l(k)$ .
11. Consider the scattering produced by a central, real potential. Assume that a large s-wave phase shift has been obtained and that the phase shifts with  $l \geq 1$  are known to be small. Find a way to improve on the results which only take  $\delta_0$  into account.
12. Consider the scattering of low-energy (0.7 eV) electrons by a rare gas atom. Suppose that the effective interaction acting on the projectile electron may be represented schematically by an attractive square well of strength  $V_0$  and range  $a \simeq 10^{-8}$  cm.
- a) Show that for a certain value of  $V_0$  the s-wave phase shift may be such that  $\delta_0 = \pi$ , while the higher order phase shifts are very small (Ramsauer–Townsend effect)
- b) Using the first two partial waves, discuss the corresponding expression for the total cross section.
- c) Assume now that the square well is repulsive. Show that in this case the Ramsauer–Townsend effect cannot occur.
13. Using the first Born approximation for  $\tan \delta_l$  [see eq. (8.74)], obtain the s-wave phase shift for scattering by
- a) the Yukawa potential  $U(r) = U_0 e^{-r/a}/r$ ,
- b) the “polarization” potential  $U(r) = U_0/(r^2 + d^2)^2$ , where  $d$  is a constant. (This potential plays an important role in the analysis of the elastic scattering of charged particles by atoms, as shown in Chapter 20.)
14. Use the first Born approximation for the phase shifts to study the scattering by potentials which fall off like  $1/r^n$  as  $r \rightarrow \infty$ . For what values of  $n$  is the forward differential cross section finite? For what values of  $n$  is the total cross section finite?
15. Solve the radial Schrödinger equation (4.17) for s-wave scattering by a (reduced) exponential potential  $U(r) = -U_0 \exp(-r/a)$ , with  $U_0 > 0$ . Find an expression for the  $S$ -matrix element  $S_0(k) = \exp[2i\delta_0(k)]$ . [Hint: Make a change of independent variable from  $r$  to  $x = 2aU_0^{1/2} \exp(-r/2a)$  so that eq. (4.17) reduces to the Bessel equation
- $$\frac{d^2 u_0}{dx^2} + \frac{1}{x} \frac{du_0}{dx} + \left(1 - \frac{v^2}{x^2}\right) u_0 = 0, \quad v = 2ika.]$$
16. Solve the radial Schrödinger equation (4.17) for s-wave scattering by a reduced repulsive potential of the form  $U(r) = \alpha/r^4$  ( $\alpha > 0$ ). Determine the phase shift  $\delta_0(k)$  and find the total cross section in the limit  $k \rightarrow 0$ .

[Hint: As in the preceding problem, reduce eq. (4.17) to the Bessel equation by setting  $r = i\alpha^{1/2}/x$  and  $u_0 = r^{1/2}\chi_0$ , so that

$$\frac{d^2\chi_0}{dx^2} + \frac{1}{x} \frac{d\chi_0}{dx} + \left(1 - \frac{1}{4x^2}\right)\chi_0 = 0.]$$

17. Analyze in detail the low-energy s-wave scattering by an attractive square well potential of depth  $U_0$  and range  $a$  in the vicinity of the critical value  $\lambda_0 a = \frac{1}{2}\pi$  (with  $\lambda_0 = U_0^{1/2}$ ) which produces a "zero energy resonance". In particular

a) Derive from the exact formula (4.154) an approximate expression for  $\tan \delta_0$ , valid through first order in the energy (i.e. through order  $k^2$ ), namely

$$\tan \delta_0 \simeq \{A_0 + B_0(ka)^2\}/\{C_0 + D_0(ka)^2\}. \quad (\text{I})$$

Find  $A_0$ ,  $B_0$ ,  $C_0$  and  $D_0$ .

b) Setting  $x_0^\pm = \lambda_0 a \pm \varepsilon$ , show that when  $\lambda_0 a = \frac{1}{2}\pi$  and  $\varepsilon$  is neglected with respect to one [but not with respect to  $(ka)^2$ ], one has

$$\tan \delta_0^\pm = \frac{2ka}{\pm \pi \varepsilon + (ka)^2}. \quad (\text{II})$$

c) Illustrate the two cases  $x_0 = \frac{1}{2}\pi + \varepsilon$  and  $x_0 = \frac{1}{2}\pi - \varepsilon$  ( $\varepsilon \rightarrow 0^+$ ) by plotting the exact s-wave phase shift [obtained from eq. (4.154)] and the approximate phase shift [obtained from eq. (II)] in the range  $0 \leq ka \leq 2$ . Compute for comparison the first Born approximation for  $\tan \delta_0$ . Draw also graphs of the s-wave cross section  $\sigma_0$  for the two cases  $x_0 = \frac{1}{2}\pi + \varepsilon$ ,  $x_0 = \frac{1}{2}\pi - \varepsilon$ , and in the same range  $0 \leq ka \leq 2$ .

18. Carry out an analysis similar to that of the preceding problem for p-wave scattering in the vicinity of the value  $\lambda_0 a = \pi$  for which a bound state with  $l = 1$  appears. In particular

a) Using eqs. (4.113) and (4.153), obtain through first order in the energy, the approximate expression

$$\tan \delta_1 \simeq \{A_1 + B_1(ka)^2\}/\{C_1 + D_1(ka)^2\}$$

and find  $A_1$ ,  $B_1$ ,  $C_1$  and  $D_1$ .

b) Setting  $x_0^\pm = \lambda_0 a \pm \varepsilon$ , show that when  $\lambda_0 a = \pi$  and  $\varepsilon$  is neglected with respect to one [but not with respect to  $(ka)^2$ ], one has

$$\tan \delta_1 = \frac{2}{3}(ka)^3 / \{\mp \frac{2}{3}\pi \varepsilon - (ka)^2\}.$$

c) Illustrate the two cases  $x_0 = \pi \pm \varepsilon$  ( $\varepsilon \rightarrow 0^+$ ) as in the preceding problem, for  $0 \leq ka \leq 2$ .

19. Consider the low-energy scattering by a repulsive square well. Using the two first partial waves, show that there is no resonance behaviour, as one would expect on physical grounds.

20. Assume that elastic and non-elastic collisions can occur in the scattering of particles A by particles B. Suppose that the forward ( $\theta = 0$ ) differential cross-section for elastic scattering is known [by extrapolation] to be 1.4 mb/steradian. Suppose also that one knows the ratio

$$\alpha = \frac{\operatorname{Re} f_{\text{el}}(\theta = 0)}{\operatorname{Im} f_{\text{el}}(\theta = 0)} = 0.25.$$

Obtain the total (complete) cross section.

21. Consider the scattering of thermal neutrons of energy 0.025 eV by a nucleus. Assuming that the total cross section for non-elastic processes  $\sigma_{\text{tot}}^{\text{r}}$  has been measured to give  $1.0 \times 10^{-27} \text{ cm}^2$ , obtain (i) the inelasticity factor  $\eta_0$  and (ii) upper and lower bounds for the elastic total cross section  $\sigma_{\text{tot}}^{\text{el}}$ .

22. Consider the scattering by a complex square well

$$U(r) = \begin{cases} -U_0, & r < a \\ 0, & r > a \end{cases}$$

with

$$U_0 = U_{\text{R}} + iU_{\text{I}} \quad (U_{\text{R}}, U_{\text{I}} > 0)$$

and  $U_{\text{R}}a^2 = 1$ ,  $U_{\text{I}}a^2 = 5$ . The incident wave number is such that  $ka = 0.1$ .

- a) Find the (complex) s-wave phase shift  $\delta_0$  and the inelasticity factor  $\eta_0$ .
  - b) Neglecting the contribution of other partial waves, obtain the total elastic cross section  $\sigma_{\text{tot}}^{\text{el}}$ , the total non-elastic cross section  $\sigma_{\text{tot}}^{\text{r}}$  and the total (complete) cross section  $\sigma_{\text{tot}}$ .
23. a) Obtain a Lippmann-Schwinger equation for the scattering in *one* dimension by a potential  $V(x)$ .
- b) Discuss the asymptotic form of the solution ( $x \rightarrow \pm \infty$ ) assuming that the beam is incident from the negative  $x$ -direction. Show that the analogue of the scattering amplitude in one dimension is a reflection amplitude  $R$  and a transmission amplitude  $T$ . Obtain formal expressions for  $R$  and  $T$  and derive a high-energy (Born) approximation for them. From elementary considerations one expects that  $|R|^2 + |T|^2 = 1$ . Is this the case for your Born amplitudes? Explain.
- c) Use your results to discuss the case of one-dimensional scattering by a delta-function potential  $V(x) = V_0\delta(x)$ .
24. Consider again the one-dimensional motion in a potential  $V(x)$ , but discuss now the bound-state problem by converting the Schrödinger equation into a homogeneous integral equation. In particular, apply your results to the case of an attractive delta-function potential  $V(x) = -V_0\delta(x)$  ( $V_0 > 0$ ). Find any bound states that may exist.

25. Consider the scattering by the "delta shell" potential  $U(r) = -U_0\delta(r-a)$ ,  $U_0 > 0$ . This interaction, which vanishes everywhere except on a sphere of radius  $a$  represents crudely the potential experienced by a neutron when it interacts with a nucleus of radius  $a$ . Solve the radial Lippmann-Schwinger equation (5.98) for the radial functions  $R_l(k, r)$  and obtain the quantities  $\tan \delta_l$  together with the partial wave amplitudes  $a_l(k)$ . Analyze in detail the s-wave and p-wave scattering and study the resonances.
26. Solve exactly the Lippmann-Schwinger equation (5.33) and the corresponding partial wave equations for a three-dimensional delta-function potential  $U(r) = U_0\delta(r)$ . Compare your results with those of Problem 23. Analyze also the first and second Born approximations to the scattering amplitude and comment on the applicability of perturbation theory in this case.

[Note that in polar coordinates one has

$$\delta(\mathbf{r} - \mathbf{r}') = \delta(r - r')\delta(\theta - \theta')\delta(\phi - \phi')/r^2 \sin \theta.]$$

27. Consider the elastic scattering of a carbon nucleus  $^{12}_6\text{C}$  by an oxygen nucleus  $^{16}_8\text{O}$  at a center of mass energy of 1 MeV

a) Use a simple classical argument to show that only the Coulomb interaction between the two nuclei should be taken into account. Obtain the corresponding differential cross section in the center of mass system and compute the Gamow factor.

b) Suppose that the pure Coulomb interaction  $V_c(r)$  is screened at a distance  $R_s \simeq 10^{-8}$  cm by the presence of atomic electrons and that the effective interaction is written approximately as

$$V(r) = \begin{cases} V_c(r), & r < R_s \\ 0, & r > R_s. \end{cases}$$

Give an estimate of the angular range in which this screening effect will influence the scattering.

c) Assume now that the screened Coulomb potential takes the form  $V(r) = (Z_1 Z_2 e^2/r) \exp(-r/R_s)$ . Use the first Born approximation to estimate the angular range over which the differential cross section arising from this potential differs from Rutherford scattering. Compare with the estimate obtained in (b).

28. Alpha particles of laboratory kinetic energy  $K_L = 4\text{MeV}$  are scattered elastically by copper nuclei  $^{63}_{29}\text{Cu}$ . In performing this experiment it is observed that the pure Coulomb scattering law is obeyed even for scattering in the backward direction ( $\theta = 180^\circ$  in the C.M. system). Using simple classical considerations, obtain an upper limit for the radius of the  $^{63}_{29}\text{Cu}$  nucleus.

29. Generalize the relations (4.105) and (4.106) to include the case of interactions which contain a Coulomb potential. In particular, investigate the relation between the quantities  $\delta_l$  [i.e. the phase shifts due to a short range potential in the presence of a Coulomb term] and the variation in sign of the short-range potential.
30. A spinless particle of mass  $m$ , wave number  $k$  and elementary charge  $e$  is scattered by a real central potential which consists of a strong interaction of short range  $a$  and a Coulomb potential  $e^2/r$ . Assume that the scattering occurs in an energy region where the  $l = 0$  partial wave – and only that one – is affected by the short range interaction.
  - a) Show that the sign of the phase shift  $\delta_0$  [i.e. the s-wave phase shift due to the strong interaction in the presence of the Coulomb term] may be directly determined by comparing the measured angular distribution with that predicted from pure Coulomb scattering.
  - b) In particular, suppose that the measured intensity in the backward direction is found to be somewhat smaller than the one arising from the Rutherford formula. What is the sign of  $\delta_0$ ? Is the short range force attractive or repulsive?
31. Consider the elastic scattering of two identical particles which interact through a central, spin-independent short range potential. Discuss the low energy C.M. differential cross section (and in particular the limit  $E \rightarrow 0$ )
  - a) for boson–boson scattering
  - b) for fermion–fermion scattering.
32. Two alpha particles having a center of mass energy of 1 MeV scatter elastically
  - a) Use a simple classical argument to suggest that only Coulomb forces should be taken into account at that energy.
  - b) Obtain and plot the Mott differential cross section in the C.M. system. Compare your results with those obtained (i) by ignoring the interference term (classical values) and (ii) by ignoring the fact that the two particles are identical.
33. Obtain the center of mass differential cross section for electron–electron scattering at a relative velocity  $v = 10^9$  cm/sec, assuming that the system is unpolarized. Compare your results with those obtained (i) by ignoring the interference term (classical values) and (ii) by ignoring the fact that the two particles are identical.
34. Consider proton–proton elastic scattering in the center of mass system.
  - a) Compute and plot the Mott differential cross section at an energy  $E = 50$  keV.
  - b) Justify the neglect of nuclear forces made in (a). Above what energy  $E_0$  would you expect a severe breakdown of this approximation?

c) Assume that the experiment is now carried out at an energy  $E > E_0$  and that only the  $l = 0$  phase shift is modified by the nuclear interaction. Write down an expression for the ratio of the modified differential cross section to that given by pure Mott scattering. [Note: Because of the Pauli principle only singlet spin states contribute to the scattering in the  $l = 0$  partial wave.]

35. Determine in first Born approximation the scattering amplitude, the differential and the total cross sections for the scattering by the following (reduced) potentials

a) Exponential potential  $U(r) = U_0 \exp(-\alpha r)$ .

b) Gaussian potential  $U(r) = U_0 \exp(-\alpha^2 r^2)$ .

c) Square well  $U(r) = U_0, r < a$   
 $= 0, r > a$ .

d) "Polarization" potential  $U(r) = U_0/(r^2 + d^2)^2$ .

Analyze and compare the various angular distributions with those obtained in the text for Yukawa-type potentials. Verify also explicitly that  $\sigma_{\text{tot}}^{\text{BI}} \sim A/E$  as  $E \rightarrow \infty$  and find the value of  $A$  in each particular case.

36. Using the screened Coulomb potential

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \exp(-r/R_s)$$

with  $R_s = 10^{-8}$  cm, estimate in first Born approximation the angular range over which the differential cross section differs from pure Coulomb (Rutherford) scattering

a) for a 1 MeV alpha particle scattered by a copper nucleus  ${}^{63}_{29}\text{Cu}$ ,

b) for a 1 MeV proton scattered by an oxygen nucleus  ${}^{16}_8\text{O}$ ,

c) for a 100 eV electron scattered by an oxygen nucleus  ${}^{16}_8\text{O}$ .

All energies are given in the center of mass system.

37. Study in second Born approximation the scattering by an exponential potential  $U(r) = U_0 \exp(-\alpha r)$ . [Note: Use the Dalitz integrals and the Feynman parametrization technique of Appendix D.]

38. Compute the second Born approximation for the scattering by a gaussian potential  $U(r) = U_0 \exp(-\alpha^2 r^2)$ . [Note: Perform the calculations in configuration space.]

39. Analyze the convergence of the Born series for  $\tan \delta_l$  and for the partial wave amplitudes  $a_l$  when the reduced potential is the "delta shell" interaction  $U(r) = -U_0 \delta(r - a)$ ,  $U_0 > 0$  (see Problem 25). Relate your discussion to the occurrence of bound states.

40. Use the unitarity relation (4.94) to express  $\text{Im } \tilde{f}_{Bn}$  in terms of the quantities  $\tilde{f}_{Bj}$ , with  $j < n$ . In particular, check in this way the expression of  $\text{Im } \tilde{f}_{B2}$  obtained in the text [see eq. (8.98)] for a Yukawa potential.

41. Use the eikonal approximation to obtain the total cross section for scattering by

a) A square well potential  $U(r) = \begin{cases} U_0, & r < a \\ 0, & r > a. \end{cases}$

b) A gaussian potential  $U(r) = U_0 \exp(-\alpha^2 r^2)$ .

Plot  $\sigma_{\text{tot}}$  as a function of the dimensionless parameter  $|U_0|a/2k$ . Compare with the results given by the first Born approximation.

42. Analyze in the eikonal approximation the scattering by a screened Coulomb potential

$$V(r) = V_c(r)s(r)$$

where  $V_c(r) = Z_1 Z_2 e^2/r$  is the Coulomb interaction between the incident and target particles and the screening function  $s(r)$  is given by

$$s(r) = \begin{cases} 1, & r < R_s \\ 0, & r > R_s. \end{cases}$$

Here  $R_s$  is a "large" screening distance. (Give a precise meaning to this statement.) Compare the scattering amplitude and differential cross section with those obtained in Chapter 6 for pure Coulomb scattering. How would the results be affected if the screening function were of the form  $s(r) = \exp(-r/R_s)$ ?

43. Use the eikonal approximation to study the scattering amplitude and the differential cross section corresponding to the scattering by an attractive Yukawa potential of unit "range", namely  $U(r) = -U_0 \exp(-r)/r$ ,  $U_0 > 0$ . [Note: Obtain the quantity  $f_E$  by performing a numerical integration.] Compare your eikonal results with the exact, first Born and second Born results given in Tables 8.1–8.3 for various values of  $U_0$  and  $k$ .

44. The asymptotic relation (9.84) was shown to be valid for all momentum transfers in the case of scattering by Yukawa-type potentials. By analyzing the quantities  $\text{Im } \tilde{f}_{B2}(k, \Delta)$  and  $\text{Im } \tilde{f}_{E2}(k, \Delta)$  for large  $k$  in the forward and backward direction, what can you say about the validity of such an asymptotic relation for

a) an exponential potential  $U(r) = U_0 \exp(-\alpha r)$ ,

b) a gaussian potential  $U(r) = U_0 \exp(-\alpha^2 r^2)$ ,

c) a polarization potential  $U(r) = U_0/(r^2 + d^2)^2$ ?

45. Use the eikonal approximation and the method of stationary phases to analyze the angular distribution for quasi-classical scattering by a

(reduced) potential having the form  $U(r) = U_0/r^s$  ( $s > 2$ ) at large distances. Prove that the total cross section is given by

$$\sigma_{\text{tot}} = 2(\pi)^{s/(s-1)} \sin \left[ \frac{\pi}{2} \left( \frac{s-3}{s-1} \right) \right] \Gamma \left( \frac{s-3}{s-1} \right) \left\{ \frac{\Gamma[\frac{1}{2}(s-1)]}{\Gamma(\frac{1}{2}s)} \right\}^{2/(s-1)} \left( \frac{U_0}{2k} \right)^{2/(s-1)}$$

where  $\Gamma$  is the Euler gamma function. Obtain also the eikonal phase shifts (9.46) and show that they lead to the same expression for  $\sigma_{\text{tot}}$  when substituted in the partial wave series (4.71).

46. Prove that for a scattering potential  $U(r) = U_0/r^2$  ( $U_0 > 0$ ), the WKB phase shifts  $\delta_l^{\text{WKB}}$  give the exact values of  $\delta_l$  (obtained in Problem 1).
47. Consider the scattering of a particle by an attractive "polarization" potential of the form  $U(r) = -U_0/(r^2 + d^2)^2$ , with  $d = 1$  (unit of length). The wave number is  $k = 5$ . Obtain the WKB phase shifts  $\delta_l^{\text{WKB}}$  for  $0 \leq l \leq 10$  and for the potential "strengths"  $U_0 = 1$  and  $U_0 = 250$ . Check your results against those of Table 9.7. Compare with the first Born values of the phase shifts obtained by using eq. (8.74).
48. Consider the scattering by an attractive square well potential of strength  $U_0$  and range  $a$ . Calculate the scattering length as a function of the quantity  $\beta = U_0^{1/2}a$ .

a) By using the Hulthén-Kohn variational method with s-wave trial wave functions of the form (10.34), namely

$$u^0(r) = \begin{cases} \sum_{i=1}^N c_i r^i, & r < a \quad (N = 1, 2, 3, 4) \\ \alpha - r, & r > a. \end{cases}$$

Check that the minimum principle (10.103) is verified when the potential cannot support a bound state.

b) By using the bilinear form of the Schwinger variational principle for  $k \cot \delta_0$ , with trial wave functions of the form

$$u^0(r) = \sum_{i=1}^N c_i r^i, \quad r < a \quad (N = 1, 2, 3, 4).$$

Compare your results with the exact values  $\bar{\alpha}$  and those of other approximations, as given in Table 10.3.

49. Consider the s-wave scattering by an exponential potential

$$U(r) = -U_0 \exp(-r/a)$$

[with  $a = 1$  and  $U_0 = 2.5$ ], at an incident wave number such that  $ka = 0.25$ . Obtain the quantity  $\lambda_0 = \tan \eta_0$  ( $= \tan \delta_0$ ) by using the Hulthén-Kohn variational method with trial wave functions of the form

$$u_0(r) = \sin kr + \lambda_0 \cos kr(1 - e^{-\kappa r}) + e^{-\kappa r} \sum_{i=1}^N c_i r^i \quad (N = 1, 2, 3).$$



Perform the variational calculation for a fixed value of the non-linear parameter  $\kappa$  and then let  $\kappa$  vary from 0.5 to 10 in discrete steps. [Note: The exact value of  $\lambda_0$  is  $-1.9900$ .]

50. Consider the s-wave scattering by a Yukawa potential of the form  $U(r) = -U_0 \exp(-r/a)/r$  [with  $a = 1$  and  $U_0 = -2$ ] at an incident wave number such that  $ka = 1$ . Obtain the quantity  $\lambda_0 = \tan \eta_0$  by using the bilinear form of the Schwinger variational principle with trial wave functions of the type

$$u_0(r) = e^{-\kappa r} \sum_{i=1}^N c_i r^i \quad (N = 1, 2).$$

Perform first the calculations for the value  $\kappa = 1$  of the non-linear parameter. Then let  $\kappa$  vary and investigate the effects of this variation on the variational results. Discuss. [Note: The exact value of  $\lambda_0$  is 1.93.]

51. Use the simplified form (10.68) of Schwinger's fractional variational principle to study the scattering by a Yukawa potential

$$U(r) = -U_0 \exp(-r/a)/r,$$

with  $U_0 = a = 1$ . Perform your calculations for  $ka = 1, 3, 5$  and compare the Schwinger differential cross sections with the first Born, second Born and exact results given in Table 8.1. Discuss. [Note: The expressions of  $f_{B1}$  and  $f_{B2}$  which you need are given in Section 8.6.1.]

52. Determine the Jost function for p-wave ( $l = 1$ ) scattering by an attractive square well potential. Analyze its analytic properties and relate your discussion to the bound state problem.
53. Obtain the Jost function  $f(k)$  for s-wave scattering by an exponential potential  $U(r) = -U_0 \exp(-r/a)$ ,  $U_0 > 0$ . Discuss the analytic properties of  $f(k)$  and of the  $S$ -matrix  $S_0(k)$ , together with the occurrence of bound states. [Note: As in Problem 15, make the change of variables from  $r$  to  $x = 2aU_0^{1/2} \exp(-r/2a)$  in the radial equation (4.17).]

54. Study the analytic properties of the s-wave ( $l = 0$ ) partial wave amplitude corresponding to the scattering by a delta shell potential

$$U(r) = -U_0 \delta(r - a), \quad U_0 > 0$$

(i) in the complex  $k$ -plane and (ii) in the complex  $E$ -plane.

5. We have obtained in eq. (6.59) the "Coulomb  $S$ -matrix element" $^5$   $S_f = \exp(2i\sigma_l) = \Gamma(l + 1 + i\gamma)/\Gamma(l + 1 - i\gamma)$ . Use this result to obtain the bound states in an attractive Coulomb potential  $V_c = Z_1 Z_2 e^2/r$  with  $Z_1 Z_2 < 0$ .

56. Consider a Regge trajectory which produces a bound state of near zero binding energy and angular momentum  $l = 0$ . Suppose further that this

Regge trajectory is also known to cause a p-wave ( $l = 1$ ) resonance of very low energy  $E_r$  and width  $\Gamma$ .

a) Assuming that the trajectory may be approximated by a straight line, obtain its slope in terms of known quantities.

b) Proceeding further with the straight line assumption, predict the energy and the width of the next resonance.

57. Starting from the expression of the Coulomb  $S$ -matrix [see eq. (6.59)], discuss the Regge trajectories for a Coulomb potential.

58. Consider the scattering by an attractive Yukawa potential

$$U(r) = -U_0 \exp(-r/a)/r \quad (U_0 > 0)$$

whose "range"  $a$  is known. Furthermore, one also knows the scattering length  $\alpha$ , and the total cross section  $\sigma_{\text{tot}}$ . Assuming that this potential cannot support a bound state, use the dispersion relation (11.229) to compute  $U_0$  from the known quantities.

59. Consider the scattering by an interaction potential  $U(r)$  which supports no bound states and is such that the dispersion relation (11.229) may be used. Suppose that (i) a sharp p-wave resonance occurs at a low energy  $E_r$  with a narrow width  $\Gamma$ , (ii) the s-wave is the only other partial wave which contributes significantly to the scattering and (iii) the scattering length  $\alpha$  is known. Express the dispersion relation (11.229) in terms of the known quantities.

60. Use the effective range formula (11.290) to compute the quantity  $k \cot \delta_0(k)$  corresponding to the scattering by an attractive square well potential of range  $a = 1$  and "strength"  $U_0 = 2$  at a wave number  $k$  such that  $ka = 0.2$ . Compare with the exact result.

61. Show that for a polarization potential of the type  $U(r) = -U_0/(r^2 + d^2)^2$ , the effective range integral (11.291) diverges because  $u^0$  does not tend to  $v^0$  sufficiently rapidly at large distances. [Note: Investigate the large distance behaviour of  $u^0$  by using a power series development of the type

$$u^0 \sim r^s(1 + c_1 r^{-1} + c_2 r^{-2} + c_3 r^{-3} + \dots)]$$

62. Consider the low-energy scattering by a polarization potential of the form  $U(r) = -U_0/(r^2 + d^2)^2$  ( $U_0 > 0$ ).

a) Assuming the potential to be sufficiently "weak", use the Born approximation for  $\tan \delta_0$  to obtain an expansion through order  $k^2$  for the quantity  $k \cot \delta_0(k)$ . Comment on the differences between your results and those corresponding to the scattering by short range potentials.

b) Would you expect to find these deviations through order  $k^2$  for a potential of the form  $U(r) = -U_0/(r^2 + d^2)^3$  ( $U_0 > 0$ )?

- c) Note that for the polarization potential the quantity  $k \cot \delta_0(k)$  is an analytic function of  $k$  in Born approximation, while the correct expansion of  $k \cot \delta_0(k)$  contains terms of the type  $k^2 \log k$ . Can you suggest where such terms might come from?
63. Obtain the effective range expansion of  $k \cot \delta_0(k)$  for a delta shell potential  $U(r) = -U_0 \delta(r-a)$ ,  $U_0 > 0$ . Show that the effective range  $r_e$  is always positive in this case.
64. Find the effective range expansion of  $k \cot \delta_0(k)$  for the non-local separable Yamaguchi potential defined in Section 8.6.3.
65. Obtain the time-dependent Green's function  $K_0(x, t; x', t')$  and write down the integral equation for the scattering in *one* dimension by a time-dependent potential  $V(x, t)$ . Show that this equation reduces to the Lippmann-Schwinger equation of Problem 23 when the potential is time-independent.

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## **PART III**

### **GENERAL SCATTERING THEORY**

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# Quantum Dynamics

In this chapter we want to study the dynamics of quantum systems from a general point of view. The required formalism is first presented in Section 3.1 within the framework of the *Schrödinger picture*. Particular attention is devoted to the *evolution operator*, which will play an important role in the following chapters. The *Heisenberg picture* is studied in Section 13.2, while the *interaction picture* is analyzed in Section 13.3. As an introduction to some general methods used in quantum field theory, we conclude this chapter by a discussion of the *Dyson [1] perturbation expansion* for the evolution operator.

## 13.1. The Schrödinger picture

It is a postulate of quantum mechanics that the state of a physical system at a given instant  $t$  is completely specified by the knowledge of the *state vector*  $\Psi(t)$  at that time [2]. The necessary dynamical principle to study the time development of the system is provided by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi_s(t) = H_s \Psi_s(t) \quad (13.1)$$

where  $H_s$  is the Hamiltonian or energy operator, whose existence is implied by eq. (13.1). The subscript  $s$  indicates that eq. (13.1) is written in the *Schrödinger picture*. In that picture, the observables or dynamical variables are represented by Hermitian operators, which are time-independent, except for a possible explicit dependence on time. For example, let us select

within the Schrödinger picture the *coordinate representation* (configuration space). This corresponds to the familiar wave mechanics version of the quantum theory (see Appendix A). The basic coordinate and momentum operators of a particle are then respectively given by

$$\begin{aligned} \mathbf{r} &\rightarrow \mathbf{r}_{\text{op}} = \text{multiplication by } \mathbf{r} \\ \mathbf{p} &\rightarrow \mathbf{p}_{\text{op}} = -i\hbar \nabla_{\mathbf{r}} \end{aligned}$$

and are obviously time-independent. A time-dependent (local) potential  $V$ , however, is represented by an operator

$$V \rightarrow V_{\text{cp}}(\mathbf{r}, t)$$

which exhibits its explicit time-dependence. Similarly, in the *momentum representation*, we have

$$\begin{aligned} \mathbf{r} &\rightarrow \mathbf{r}_{\text{op}} = i\hbar \nabla_{\mathbf{p}} \\ \mathbf{p} &\rightarrow \mathbf{p}_{\text{op}} = \text{multiplication by } \mathbf{p} \end{aligned}$$

and

$$V \rightarrow V_{\text{op}}(i\hbar \nabla_{\mathbf{p}}, t).$$

Consider now an observable  $\mathcal{A}$  to which corresponds an operator  $A_s$  in the Schrödinger picture. The expectation value of  $A_s$  is defined by

$$\langle A_s \rangle = \langle \Psi_s | A_s | \Psi_s \rangle. \quad (13.2)$$

Therefore, using the Schrödinger equation (13.1), we have

$$\begin{aligned} i\hbar \frac{d}{dt} \langle A_s \rangle &= \left\langle -i\hbar \frac{\partial \Psi_s}{\partial t} \middle| A_s \middle| \Psi_s \right\rangle + \left\langle \Psi_s \middle| i\hbar \frac{\partial A_s}{\partial t} \middle| \Psi_s \right\rangle + \left\langle \Psi_s \middle| A_s \middle| i\hbar \frac{\partial \Psi_s}{\partial t} \right\rangle \\ &= \langle -H_s \Psi_s | A_s | \Psi_s \rangle + i\hbar \left\langle \Psi_s \middle| \frac{\partial A_s}{\partial t} \middle| \Psi_s \right\rangle + \langle \Psi_s | A_s | H_s \Psi_s \rangle \end{aligned}$$

or

$$i\hbar \frac{d}{dt} \langle A_s \rangle = \langle \Psi_s | [A_s, H_s] | \Psi_s \rangle + i\hbar \left\langle \Psi_s \middle| \frac{\partial A_s}{\partial t} \middle| \Psi_s \right\rangle \quad (13.3)$$

an equation which governs the time evolution of the expectation value  $\langle A_s \rangle$ . In particular, we note that if the operator  $A_s$  does not depend explicitly on time (i.e. if  $\partial A_s / \partial t = 0$ ), the necessary and sufficient condition for the observable to be a *constant of the motion* is that

$$[A_s, H_s] = 0. \quad (13.4)$$

While the basic operators are time-independent in the Schrödinger picture, the state vector  $\Psi_s(t)$ , on the contrary, evolves in time according to the Schrödinger equation (13.1). Since this is a first order differential equation in time, the state vector will be determined for all  $t$  once the state of the system is specified at any given time. It is convenient to introduce an evolution operator  $U_s(t, t_0)$  such that

$$\Psi_s(t) = U_s(t, t_0) \Psi_s(t_0). \quad (13.5)$$



Then, from eq. (13.1)

$$i\hbar \frac{\partial}{\partial t} U_s(t, t_0) = H_s U_s(t, t_0) \quad (13.6)$$

with the initial condition

$$U_s(t_0, t_0) = I \quad (13.7)$$

where  $I$  is the unit operator. Applying twice the definition (13.5) we also obtain

$$U_s(t, t_0) = U_s(t, t') U_s(t', t_0) \quad (13.8)$$

and

$$U_s^{-1}(t, t_0) = U_s(t_0, t) \quad (13.9)$$

so that the evolution operator exhibits the *group property*.

The differential equation (13.6), together with the initial condition (13.7) may be replaced by an integral equation of the Volterra type, namely

$$U_s(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^t H_s U_s(t', t_0) dt'. \quad (13.10)$$

Conservation of probability requires that

$$\langle \Psi_s(t) | \Psi_s(t) \rangle = \langle \Psi_s(t_0) | \Psi_s(t_0) \rangle. \quad (13.11)$$

However, from eq. (13.5),

$$\begin{aligned} \langle \Psi_s(t) | \Psi_s(t) \rangle &= \langle U_s(t, t_0) \Psi_s(t_0) | U_s(t, t_0) \Psi_s(t_0) \rangle \\ &= \langle \Psi_s(t_0) | U_s^\dagger(t, t_0) U_s(t, t_0) | \Psi_s(t_0) \rangle \end{aligned}$$

where the dagger denotes the Hermitian conjugate (or adjoint) operator. Therefore

$$U_s^\dagger(t, t_0) U_s(t, t_0) = I. \quad (13.12)$$

Similarly, starting from  $\langle \Psi_s(t_0) | \Psi_s(t_0) \rangle$ , we obtain

$$U_s(t, t_0) U_s^\dagger(t, t_0) = I \quad (13.13)$$

so that, from eqs. (13.12)–(13.13), we conclude that  $U_s(t, t_0)$  is a *unitary* operator.

The unitary character of the evolution operator  $U_s$  is clearly connected to the hermiticity of the Hamiltonian, which implies the conservation of probability. Let us exhibit this connection by studying the change in  $U_s$  induced after an arbitrarily small time  $\delta t$ . We first have from eq. (13.6)

$$i\hbar [U_s(t_0 + \delta t, t_0) - U_s(t_0, t_0)] = H_s U_s(t_0 + \delta t, t_0) \delta t.$$

Then, to first order in  $\delta t$ , and using eq. (13.7), we find that

$$U_s(t_0 + \delta t, t_0) = I - \frac{i}{\hbar} H_s \delta t \quad (13.14)$$

from which we deduce that if  $U_s$  is a unitary operator,  $H_s$  must be Hermitian and vice-versa. The Hamiltonian  $H_s$  is therefore the generator of an infinitesimal unitary transformation – in fact an infinitesimal time translation – described by the evolution operator  $U_s(t_0 + \delta t, t_0)$ .

As an example, let us suppose that the Hamiltonian  $H_s$  is time-independent. We then obtain from eqs. (13.6) and (13.7)

$$U_s(t, t_0) = \exp\left\{-\frac{i}{\hbar}H_s(t - t_0)\right\} \quad (13.15)$$

or

$$\Psi_s(t, t_0) = \exp\left\{-\frac{i}{\hbar}H_s(t - t_0)\right\}\Psi_s(t_0). \quad (13.16)$$

### 13.2. The Heisenberg picture

State vectors and operators are not directly accessible to observation. Indeed, let us suppose that the operator  $A$ , corresponding to the observable  $\mathcal{A}$ , has a spectrum of eigenvalues  $\alpha_n$  with corresponding eigenvectors  $|a_n\rangle$ , i.e.

$$A|a_n\rangle = \alpha_n|a_n\rangle. \quad (13.17)$$

Then, if the system under consideration is described before the measurement by a state vector  $|\Psi\rangle$ , and if a measurement is made to determine the observable  $\mathcal{A}$ , the probability of finding the value  $\alpha_n$  is given by  $|\langle a_n|\Psi\rangle|^2$ . Therefore, any new picture obtained from the Schrödinger picture by a transformation of the vectors and operators such that

- i) the eigenvalue spectrum of the operators is unchanged,
  - ii) the scalar product of the state vector with the eigenvectors is unaltered,
- is an equally acceptable formulation of the quantum theory.

These conditions are easily seen to be satisfied by a *unitary transformation*. Indeed, let  $A$  be an operator such that

$$A|x\rangle = |y\rangle \quad (13.18)$$

where  $|x\rangle$  and  $|y\rangle$  are two vectors in Hilbert space. Let  $U$  be a unitary operator which associates with each vector  $|x\rangle$  a vector  $|x'\rangle$ . Thus

$$|x'\rangle = U|x\rangle \quad ; \quad \langle x'| = \langle x|U^\dagger. \quad (13.19)$$

Similarly

$$|y'\rangle = U|y\rangle \quad ; \quad \langle y'| = \langle y|U^\dagger. \quad (13.20)$$

Let  $A'$  be the operator such that

$$|y'\rangle = A'|x'\rangle. \quad (13.21)$$

Then

$$A'U|x\rangle = U|y\rangle = UA|x\rangle$$

so that

$$U^{-1}A'U = A; \quad A' = UAU^{-1} \quad (13.22)$$

or, since  $U$  is unitary ( $U^{-1} = U^\dagger$ )

$$U^\dagger A'U = A; \quad A' = UAU^\dagger. \quad (13.23)$$

The eigenvalue equation

$$A|a_n\rangle = \alpha_n|a_n\rangle \quad (13.24)$$

can be written as

$$UAU^\dagger U|a_n\rangle = \alpha_n|a'_n\rangle$$

where  $|a'_n\rangle = U|a_n\rangle$  and we have used the fact that  $U^\dagger U = I$ . Using eq. (13.23) we then find that

$$A'|a'_n\rangle = \alpha_n|a'_n\rangle \quad (13.25)$$

so that the eigenvalues of  $A'$  are identical to those of  $A$  in agreement with condition (i). Condition (ii) is easily seen to be satisfied since

$$\langle a'_n|\Psi'\rangle = \langle a_n|U^\dagger U|\Psi\rangle = \langle a_n|\Psi\rangle. \quad (13.26)$$

There are infinitely many ways of choosing the unitary operator  $U$ , leading to an infinite number of pictures in which quantum dynamics can be formulated. The *Heisenberg picture* is obtained from the Schrödinger picture by choosing the operator  $U$  to be given by

$$U = U_s^\dagger(t, t_0) = U_s(t_0, t). \quad (13.27)$$

Thus the state vector  $\Psi_H$  in the Heisenberg picture is obtained from  $\Psi_s(t)$  as

$$\Psi_H = U_s^\dagger(t, t_0)\Psi_s(t) \quad (13.28)$$

or

$$\Psi_H = U_s(t_0, t)\Psi_s(t) = \Psi_s(t_0). \quad (13.29)$$

Hence, in the Heisenberg picture, the state vector is *fixed* in time. On the contrary, we see from eq. (13.23) that an operator  $A_s$  of the Schrödinger picture is now given in the Heisenberg picture by

$$A_H(t) = U_s^\dagger(t, t_0)A_s U_s(t, t_0) \quad (13.30)$$

and is therefore time-dependent even if  $A_s$  does not depend on time. Thus

$$i\hbar \frac{d}{dt} A_H(t) = i\hbar \frac{\partial U_s^\dagger}{\partial t} A_s U_s + i\hbar U_s^\dagger \frac{\partial A_s}{\partial t} U_s + i\hbar U_s^\dagger A_s \frac{\partial U_s}{\partial t}. \quad (13.31)$$

But, from eq. (13.6)

$$i\hbar \frac{\partial}{\partial t} U_s = H_s U_s \quad ; \quad -i\hbar \frac{\partial}{\partial t} U_s^\dagger = U_s^\dagger H_s$$

so that we may rewrite eq. (13.31) as

$$\begin{aligned} i\hbar \frac{d}{dt} A_H(t) &= -U_s^\dagger H_s A_s U_s + i\hbar U_s^\dagger \frac{\partial A_s}{\partial t} U_s + U_s^\dagger A_s H_s U_s \\ &= -U_s^\dagger H_s U_s U_s^\dagger A_s U_s + i\hbar U_s^\dagger \frac{\partial A_s}{\partial t} U_s + U_s^\dagger A_s U_s U_s^\dagger H_s U_s. \end{aligned} \quad (13.32)$$

Defining the Heisenberg operators

$$H_H = U_s^\dagger H_s U_s \quad (13.33a)$$

and

$$\frac{\partial A_H}{\partial t} = U_s^\dagger \frac{\partial A_s}{\partial t} U_s \quad (13.33b)$$

we obtain

$$i\hbar \frac{d}{dt} A_H(t) = -H_H A_H + A_H H_H + i\hbar \frac{\partial A_H}{\partial t}. \quad (13.34)$$

Introducing the commutator  $[A_H, H_H] = A_H H_H - H_H A_H$ , we may also rewrite eq. (13.34) as

$$i\hbar \frac{d}{dt} A_H(t) = [A_H, H_H] + i\hbar \frac{\partial A_H}{\partial t} \quad (13.35)$$

which is the *Heisenberg equation of motion* for the operator  $A_H$ .

The Heisenberg picture corresponds to a formulation of quantum dynamics which is formally close to classical mechanics. Indeed, if the Hamiltonian is given in terms of the canonical variables  $q_{iH}$  and  $p_{iH}$ , we may write from eq. (13.35)

$$\frac{dq_{iH}}{dt} = (i\hbar)^{-1} [q_{iH}, H_H] \quad (13.36a)$$

and

$$\frac{dp_{iH}}{dt} = (i\hbar)^{-1} [p_{iH}, H_H]. \quad (13.36b)$$

Let us now evaluate the right-hand side of eqs. (13.36). By using repeatedly the basic commutation relations

$$[q_{iH}, p_{kH}] = i\hbar \delta_{ik} \quad (13.37)$$

one obtains [3] the operator equations

$$\frac{dq_{iH}}{dt} = \frac{\partial H_H}{\partial p_{iH}} \quad (13.38a)$$

$$\cdot \quad \frac{dp_{iH}}{dt} = -\frac{\partial H_H}{\partial q_{iH}} \quad (13.38b)$$

which are formally identical to Hamilton's canonical equations in classical mechanics.

The expectation values of operators in the Heisenberg picture are given by

$$\langle A_H \rangle = \langle \Psi_H | A_H | \Psi_H \rangle. \quad (13.39)$$

They are clearly identical to those calculated in the Schrödinger picture since, using eqs. (13.28) and (13.30),

$$\begin{aligned}\langle A_H \rangle &= \langle \Psi_s | U_s U_s^\dagger A_s U_s U_s^\dagger | \Psi_s \rangle \\ &= \langle \Psi_s | A_s | \Psi_s \rangle = \langle A_s \rangle.\end{aligned}\quad (13.40)$$

We now turn to the calculation of *transition probabilities* which play a crucial role in collision theory. Let us assume that the system is at time  $t_0$  in an eigenstate  $|a\rangle$  of the operator  $A$ . We would like to calculate the probability of finding the system at time  $t$  in an eigenstate  $|b\rangle$  of the operator  $B$ . Using first the Schrödinger picture, we find that the system is at time  $t$  in the state  $U_s(t, t_0)|a_s\rangle$  so that the required probability is given by

$$|\langle b_s | U_s(t, t_0) | a_s \rangle|^2. \quad (13.41)$$

In the Heisenberg picture the state vector is and remains  $|a_s\rangle$  and the transition probability is given by

$$|\langle b_H | a_s \rangle|^2 = |\langle b_s | U_s(t, t_0) | a_s \rangle|^2 \quad (13.42)$$

as expected.

We have already seen that the Heisenberg picture emphasizes the correspondence between a quantum system and its classical analogue – if it exists. Another advantage of the Heisenberg picture over the Schrödinger picture is that the time and space dependence of the Heisenberg operators are treated on the same footing. This allows directly for covariant relativistic descriptions, so that the Heisenberg picture is particularly convenient to discuss relativistic field theories. On the other hand, we must solve in this picture a different equation for each operator. The Schrödinger picture, which we used in Part II, corresponds to a more intuitive expression of quantum dynamics, especially when formulated in the coordinate or momentum representations.

### 13.3. The interaction picture

Among the infinite number of alternative pictures in which quantum dynamics can be formulated, the *interaction picture* is particularly convenient to study collision processes; this picture also played an important role in field theory [1, 4–8].

Suppose that the Hamiltonian  $H_s$  may be split into an “unperturbed” part  $H_0$  and a “perturbation”  $V$ , namely

$$H_s = H_0 + V. \quad (13.43)$$

We assume that  $H_0$  is time-independent. Its eigenstates are the free (unperturbed) solutions  $\Phi_\alpha$  such that

$$H_0 \Phi_\alpha = E_\alpha \Phi_\alpha. \quad (13.44)$$

The subscript  $\alpha$  refers to all the information on the state obtained by adding to  $H_0$  a complete set of commuting observables.

We now wish to separate the free motion from the motion of the total system. To do this, we make on the Schrödinger state vector  $\Psi_s(t)$  the unitary transformation [9]

$$\Psi(t) = \exp\{iH_0(t - t_0)\}\Psi_s(t) \quad (13.45)$$

which defines the new state vector  $\Psi(t)$  in the interaction picture. From eq. (13.1) we obtain for  $\Psi(t)$  the *Tomonaga-Schwinger* equation [4, 5]

$$i \frac{\partial \Psi(t)}{\partial t} = V(t)\Psi(t) \quad (13.46)$$

where

$$V(t) = \exp\{iH_0(t - t_0)\}V\exp\{-iH_0(t - t_0)\}. \quad (13.47)$$

Therefore the state vector  $\Psi(t)$  is time-dependent, but *this dependence is entirely due to the interaction*. On the other hand, the observables are represented by operators whose equations of motion only contain the “unperturbed” Hamiltonian  $H_0$ . Indeed, a calculation similar to the one leading to eq. (13.35) yields

$$i \frac{dA(t)}{dt} = [A, H_0] + i \frac{\partial A}{\partial t} \quad (13.48)$$

where

$$A(t) = \exp\{iH_0(t - t_0)\}A_s\exp\{-iH_0(t - t_0)\} \quad (13.49)$$

and

$$\frac{\partial A}{\partial t} = \exp\{iH_0(t - t_0)\} \frac{\partial A_s}{\partial t} \exp\{-iH_0(t - t_0)\}. \quad (13.50)$$

We note that these equations are identical to those obtained in the Heisenberg picture, but *without the interaction*. The interaction picture is therefore intermediate between the Schrödinger and the Heisenberg pictures: both the state vector and the observables change in time. However, the kinematical and dynamical evolution of the system are nicely separated. Indeed, the evolution of the observables only depends on  $H_0$  and is therefore purely kinematical, while the evolution of the state vector is controlled by the interaction. This separation is particularly convenient in the analysis of collision phenomena.

Expectation values of operators in the interaction picture are given by

$$\langle A \rangle = \langle \Psi(t) | A(t) | \Psi(t) \rangle \quad (13.51)$$

and are of course identical to those calculated in the Schrödinger and Heisenberg pictures. We also note that the Schrödinger, Heisenberg and interaction pictures coincide at the time  $t = t_0$ . One generally chooses  $t_0 = 0$  or  $t_0 = -\infty$ .

We now define an *evolution operator* in the interaction picture by the equation

$$\Psi(t) = U(t, t')\Psi(t'). \quad (13.52)$$

As in the case of the operator  $U_s$  introduced previously, we have

$$\begin{aligned} U(t, t) &= I \\ U(t, t') &= U(t, t'')U(t'', t') \end{aligned} \quad (13.53)$$

and

$$U^{-1}(t, t') = U(t', t).$$

The Tomonaga–Schwinger equation (13.46) can be written as

$$i \frac{\partial}{\partial t} U(t, t') \Psi(t') = V(t) U(t, t') \Psi(t') \quad (13.54)$$

and since it is valid for all  $t'$ , we deduce that

$$i \frac{\partial}{\partial t} U(t, t') = V(t) U(t, t'). \quad (13.55)$$

This last equation, together with the initial condition  $U(t, t) = I$  can be summarized in one integral equation of the Volterra type, namely

$$U(t, t') = I - i \int_{t'}^t V(t_1) U(t_1, t') dt_1. \quad (13.56)$$

As in the case of the operator  $U_s$ , one can show that  $U$  is a *unitary* operator. That is,

$$U^\dagger(t, t') = U^{-1}(t, t') = U(t', t). \quad (13.57)$$

Therefore, returning to eq. (13.56), we deduce that

$$U(t', t) = I + i \int_{t'}^t U(t', t_1) V(t_1) dt_1$$

or, by permutation of  $t$  and  $t'$ ,

$$U(t, t') = I + i \int_t^{t'} U(t, t_1) V(t_1) dt_1. \quad (13.58)$$

What is the connection between the evolution operators  $U_s$  and  $U$ ? We have from eqs. (13.45) and (13.5)

$$\begin{aligned} \Psi(t) &= \exp\{iH_0(t - t_0)\} \Psi_s(t) \\ &= \exp\{iH_0(t - t_0)\} U_s(t, t') \Psi_s(t') \end{aligned}$$

or

$$\Psi(t) = \exp\{iH_0(t - t_0)\} U_s(t, t') \exp\{-iH_0(t' - t_0)\} \Psi(t'). \quad (13.59)$$

Comparing eq. (13.59) with eq. (13.52), we obtain

$$U(t, t') = \exp\{iH_0(t - t_0)\} U_s(t, t') \exp\{-iH_0(t' - t_0)\}. \quad (13.60)$$

If we choose  $t_0 = 0$ , this becomes

$$U(t, t') = \exp(iH_0 t) U_s(t, t') \exp(-iH_0 t'). \quad (13.61)$$

Finally, in the particular case where the total Hamiltonian is time-independent, we may use eq. (13.15) to obtain from eq. (13.61)

$$U(t, t') = \exp(iH_0 t) \exp\{-iH_s(t - t')\} \exp(-iH_0 t'). \quad (13.62)$$

### 13.4. Dyson's perturbation expansion for the evolution operator

Let us attempt to solve the integral equation (13.56) by iteration [10] in order to generate an expansion of the evolution operator  $U$  in powers of the interaction  $V$ . We start from the zero order approximation

$$U^{(0)}(t, t') = I. \quad (13.63)$$

The first order approximation is then

$$U^{(1)}(t, t') = I - i \int_{t'}^t V(t_1) dt_1. \quad (13.64)$$

Similarly, we have to second order in  $V$

$$U^{(2)}(t, t') = I - i \int_{t'}^t V(t_1) dt_1 + (-i)^2 \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 V(t_1)V(t_2). \quad (13.65)$$

Assuming that the sequence  $U^{(0)}, U^{(1)}, U^{(2)}, \dots$  converges towards the evolution operator  $U$ , we may then write

$$U(t, t') = \sum_{n=0}^{\infty} U_n(t, t') \quad (13.66)$$

where  $U_0(t, t') = I$  while for  $n \geq 1$

$$U_n(t, t') = (-i)^n \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 \dots \int_{t'}^{t_{n-1}} dt_n V(t_1)V(t_2) \dots V(t_n). \quad (13.67)$$

If we choose  $t' < t$  it is clear that the ordering

$$t' \leq t_n \leq t_{n-1} \dots \leq t_1 \leq t \quad (13.68)$$

is imposed. This ordering is important since in general the operators  $V(t_i)$  and  $V(t_j)$  do not commute. This critical time-ordering and the fact that the upper limits of integration in eq. (13.67) are not equal complicate the evaluation of  $U_n(t, t')$ .

In order to formally avoid these difficulties, Dyson [1] has proposed the following procedure. A *chronological ordering operator*  $P$  is introduced, such that

$$P[A(t_1)B(t_2)] = \begin{cases} A(t_1)B(t_2) & \text{if } t_1 > t_2 \\ B(t_2)A(t_1) & \text{if } t_2 > t_1 \end{cases} \quad (13.69)$$

where  $A(t)$  and  $B(t)$  are arbitrary time-dependent operators. The effect of the operator  $P$  is therefore to order the factors so that the time arguments of the operators decrease from left to right. This definition can be generalized to a product of  $n$  operators,

$$P[A_i(t_i)A_j(t_j) \dots A_k(t_k)] = A_1(t_1)A_2(t_2) \dots A_n(t_n) \quad \text{with } t_1 > t_2 > \dots > t_n. \quad (13.70)$$

The possible ambiguity which could arise when  $t_i = t_j$  does not occur in our case since we have  $A_1 = A_2 = \dots = A_n = V$  at equal times.



Having defined the operator  $P$ , we now consider the expression

$$U_2(t, t') = (-i)^2 \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 V(t_1) \dot{V}(t_2) \quad (13.71)$$

which occurs in eq. (13.65). In the  $(t_1, t_2)$  plane, the region of integration in eq. (13.71) is clearly a triangle below the bisector of the angle between the coordinate axes (see Fig. 13.1). Now, if we interchange the names of the integration variables  $t_1$  and  $t_2$  in eq. (13.71), we obtain

$$U_2(t, t') = (-i)^2 \int_{t'}^t dt_2 \int_{t'}^{t_2} dt_1 V(t_2) V(t_1). \quad (13.72)$$

In the  $(t_1, t_2)$  plane, the region of integration now becomes a triangle above the bisector of the coordinate angle, while the integrand differs from that in eq. (13.71) by the order of the factors. If  $V(t_1)$  and  $V(t_2)$  would commute, then  $U_2(t, t')$  would simply be half the integral over the whole square.

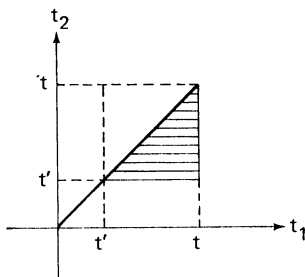


Fig. 13.1. Illustration of integration regions in the  $(t_1, t_2)$  plane. The shaded triangle is the integration domain for eq. (13.71). The unshaded triangle above the bisector of the coordinate angle is the integration region for eq. (13.72).

Introducing the operator  $P$ , we now assert that

$$U_2(t, t') = \frac{(-i)^2}{2} \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 P[V(t_1)V(t_2)]. \quad (13.73)$$

Indeed

$$\begin{aligned} & \frac{(-i)^2}{2} \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 P[V(t_1)V(t_2)] \\ &= \frac{1}{2} \left[ (-i)^2 \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 V(t_1)V(t_2) + (-i)^2 \int_{t'}^t dt_1 \int_{t_1}^t dt_2 V(t_2)V(t_1) \right]. \end{aligned}$$

The first term in the bracket is identical to the right-hand side of eq. (13.71); the second term reduces to the right-hand side of eq. (13.72) since it corresponds to the integration of the same function over the same domain (see Fig. 13.1).

This method can be generalized to all the operators  $U_n(t, t')$ . Since there are  $n!$  permutations of the set of time variables  $t_1, t_2, \dots, t_n$ , one finds that

$$U_n(t, t') = \frac{(-i)^n}{n!} \int_{t'}^t dt_1 \int_{t'}^t dt_2 \dots \int_{t'}^t dt_n P[V(t_1)V(t_2) \dots V(t_n)]. \quad (13.74)$$

Returning to eq. (13.66) we see that

$$U(t, t') = I + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^t dt_1 \int_{t'}^t dt_2 \dots \int_{t'}^t dt_n P[V(t_1)V(t_2) \dots V(t_n)] \quad (13.75)$$

or, symbolically

$$U(t, t') = P \exp \left\{ -i \int_{t'}^t V(t'') dt'' \right\}. \quad (13.76)$$

The formula (13.76) is of course formal as long as explicit expressions of the chronological operator  $P$  are not known. We note, however, that such expressions can be obtained from the commutation relations of the operators  $V(t)$ . Thus, if the commutator

$$[V(t_1), V(t_2)] = F(t_1, t_2) \quad (13.77)$$

is known, then

$$P[V(t_1)V(t_2)] = V(t_1)V(t_2) - \Theta(t_2 - t_1)F(t_1, t_2) \quad (13.78)$$

where  $\Theta(x)$  is the step function such that

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases} \quad (13.79)$$

The generalization to more factors is straightforward. The procedure of elimination of the chronological ordering operator  $P$  is often called "reduction to normal form". This operation is particularly important in quantum field theory, where convenient techniques have been devised [7, 8].

## References and notes

- [1] DYSON, F. J. (1949), Phys. Rev. **75**, 486.
- [2] We emphasize that since the state vector is a vector in an abstract Hilbert space, all the statements which will be made hold equally well in any *representation* of the quantum theory such as the coordinate representation (configuration space), the momentum representation, the particle number representation, etc.
- [3] This may be seen as follows. If  $q_{iH}$  and  $p_{kH}$  are canonically conjugate variables which obey the commutation relations (13.37) then by induction one has

$$[q_{iH}, p_{kH}^n] = n i \hbar p_{kH}^{n-1} \delta_{ik} \quad (Ia)$$

and

$$[p_{iH}, q_{kH}^n] = - n i \hbar q_{kH}^{n-1} \delta_{ik}. \quad (Ib)$$

Consider now an observable  $\mathcal{A}$  represented by an operator  $A_H$  which is a function of the quantities  $q_{iH}$  and  $p_{iH}$ , arranged in a given order. Since any operator  $A_H$  can be represented by a power series in  $q_{iH}$  and  $p_{iH}$ , we find from eqs. (I) that

$$[q_{iH}, A_H] = i \hbar \partial A_H / \partial p_{iH} \quad (IIa)$$

and

$$[p_{iH}, A_H] = -i\hbar \partial A_H / \partial q_{iH}. \quad (\text{IIb})$$

In particular, for the case  $A_H = H_H$  one has

$$[q_{iH}, H_H] = i\hbar \partial H_H / \partial p_{iH} \quad (\text{IIIa})$$

and

$$[p_{iH}, H_H] = -i\hbar \partial H_H / \partial q_{iH}. \quad (\text{IIIb})$$

Upon substitution of eqs. (III) into eqs. (13.36) we then obtain eqs. (13.38).

- [4] TOMONAGA, S. (1946), *Prog. Theor. Phys. (Kyoto)* **1**, 27.
- [5] SCHWINGER, J. (1948), *Phys. Rev.* **74**, 1439.
- [6] JAUCH, J. M. and F. ROHRICH (1955), *The Theory of Photons and Electrons* (Addison-Wesley, Cambridge, Mass.)
- [7] BOGOLIUBOV, N. N. and D. V. SHIRKOV (1959), *Introduction to the Theory of Quantized Fields* (Interscience, New York).
- [8] SCHWEBER, S. S. (1961), *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York).
- [9] We simplify the notation by choosing  $\hbar = 1$  in what follows.
- [10] The iterative solution attempted here is known as the Liouville–Neumann series in the theory of integral equations. This series always converges for Volterra equations, provided that the objects considered are ordinary *c*-numbers. However, in our case the situation is more complicated since we are dealing with operators.

## The Collision Matrix

We now apply the formalism of Chapter 13 to analyze quantum collisions in a general way. The basic ideas used to describe the collision are simple: a beam of free particles, prepared in the *remote past*, interacts with the target and in the *far future* the detectors record the scattered particles in the asymptotic region. Therefore, we shall first study in Section 14.1 the limit of the evolution operator for infinite times. In Section 14.2 we introduce the central object of collision theory: the *S-matrix*. Section 14.3 is devoted to the study of Green's operators while the *T-matrix*, closely related to the *S-matrix*, is introduced and analyzed in Section 14.4.

### 14.1. The passage to infinite times. The Møller operators

Before we study the evolution operator for infinite times, we must first generalize the considerations developed in the preceding chapter to the case where the Hamiltonian  $H$  of the system can be decomposed in various ways as

$$H = H_c + V_c. \quad (14.1)$$

Here  $V_c$  is the interaction between the particles of channel  $c$  and  $H_c$  describes these particles when they are far apart and do not interact. Several channels may of course correspond to a given splitting (14.1) of the total Hamiltonian if they differ only by the quantum numbers of their fragments. For example, if we return to a case considered in Sections 1.1 and 1.2 the elastic channel

$$e^+ + H \rightarrow e^+ + H \quad (14.2)$$

and all the inelastic final channels

$$e^+ + H \rightarrow e^+ + H^* \quad (14.3)$$

(where  $H^*$  is an excited hydrogen atom) correspond to the initial decomposition  $H = H_i + V_i$ . Here the Hamiltonian

$$H_i = K_{e^+} + K_p + K_{e^-} + V_{pe^-} \quad (14.4)$$

is the sum of the kinetic energies of the three particles and of the proton-electron interaction  $V_{pe^-}$ , while

$$V_i = V_{e^+p} + V_{e^+e^-} \quad (14.5)$$

is the sum of the interactions between the projectile positron and the two target particles. On the contrary, in the binary rearrangement collision

$$e^+ + H \rightarrow p + (e^+e^-) \quad (14.6)$$

– where  $(e^+e^-)$  denotes a positronium atom in the ground state – the final channel  $f$  corresponds to another decomposition  $H = H_f + V_f$  of the total Hamiltonian. That is,

$$H_f = K_p + K_{e^+} + K_{e^-} + V_{e^+e^-} \quad (14.7)$$

while

$$V_f = V_{pe^+} + V_{pe^-}. \quad (14.8)$$

Clearly all the final channels corresponding to the reactions

$$e^+ + H \rightarrow p + (e^+e^-)^* \quad (14.9)$$

– where  $(e^+e^-)^*$  denotes an excited state of the positronium atom – share this decomposition of  $H$  into  $H_f$  and  $V_f$ .

The various possible splittings of  $H$ , which are determined by the number and the nature of the particles which participate in the collision, will be referred to as *arrangement channels*. Since a given decomposition (14.1) may be common to several channels, each arrangement channel may contain several ordinary channels differing by the quantum states of their fragments. Thus in the above example all the final channels corresponding to the reactions (14.6) and (14.9) belong to the arrangement channel  $f$  for which  $H_f$  and  $V_f$  are given respectively by eqs. (14.7) and (14.8).

We shall denote by  $\Phi_{c,\gamma}$  the asymptotic, “free” state vectors describing the system in the state  $\gamma$  when it is in the arrangement channel  $c$ . The subscript  $\gamma$  is a condensed notation which contains all the information about the momenta, spin, isospin, possible bound state quantum numbers, etc., of the particles when they are in the asymptotic region in channel  $c$ . The  $\Phi_{c,\gamma}$  obviously satisfy the Schrödinger equations

$$H_c \Phi_{c,\gamma} = E_{c,\gamma} \Phi_{c,\gamma}. \quad (14.10)$$

We shall use the subscript  $\alpha$  to denote the initial state of the system in the incoming arrangement channel  $i$  while  $\beta$  will refer to the final state of the system in the outgoing arrangement channel  $f$  [1]. The corresponding “free” state vectors are then respectively  $\Phi_{i,\alpha}$  and  $\Phi_{f,\beta}$ . It will sometimes prove convenient to contract somewhat this notation and define the indices  $a \equiv (i, \alpha)$ ,  $b \equiv (f, \beta)$  and  $n \equiv (c, \gamma)$  so that  $\Phi_a \equiv \Phi_{i,\alpha}$ ,  $\Phi_b \equiv \Phi_{f,\beta}$  and  $\Phi_n \equiv \Phi_{c,\gamma}$ .

It is worth noting that the asymptotic channel states  $\Phi_{c,\gamma}$  do not in general form a complete set. This is due to the fact that the ionized eigenstates of  $H_c$  are missing from the set of states  $\Phi_{c,\gamma}$ . The only exception arises when the total Hamiltonian  $H$  describes a system of  $n$  "elementary" particles, and the channel Hamiltonian is the one for which all the particles are free (i.e. the " $n$ -fragment" arrangement channel). In what follows we shall denote by  $\Phi_\xi$  the complete set of eigenvectors of  $H_c$ . The set of functions  $\Phi_\xi$  obviously includes the  $\Phi_{c,\gamma}$ .

In order to illustrate these considerations, let us consider a system made of a proton, a neutron and an electron. The various arrangement channels correspond to the situations for which one has

- i) an hydrogen atom and a free neutron:  $(p e^-) + n$ ,
- ii) a deuteron and a free electron:  $(p n) + e^-$ ,
- iii) three free particles:  $p + n + e^-$ .

Note that conservation laws forbid the formation of the bound states of deuterium in a collision involving the three particles  $p$ ,  $n$  and  $e^-$ , so that we do not call deuterium a "channel". However, these three-body bound states do enter into the formulation of the scattering problem, as we shall see below.

The arrangement channel  $(p e^-) + n$  contains an infinite number of ordinary channels labelled by the quantum states of the bound system  $(p e^-)$ . We note that the asymptotic channel states  $\Phi_{c,\gamma}$  corresponding to this arrangement channel do not form a complete set since they only describe the cases where the hydrogen atom is bound. Similarly, the channel states which correspond to the arrangement channel  $(p n) + e^-$  do not form a complete set, since they do not include the states for which the deuteron is unbound. On the other hand, the channel states  $\Phi_{c,\gamma}$  corresponding to the 3-fragment (all free) arrangement channel form a complete set.

For each arrangement channel  $c$  corresponding to a decomposition  $H = H_c + V_c$  there exists an evolution operator  $U_c(t, t')$  in the interaction picture. Now in a collision process a system, which in the remote past ( $t' \rightarrow -\infty$ ) was in the arrangement channel  $i$  and the state  $\alpha$ , is found in the far future ( $t \rightarrow +\infty$ ) in the arrangement channel  $f$  and the state  $\beta$ . It is therefore essential to examine the limit of the evolution operator  $U_c(t, t')$  for infinite arguments. This passage to infinite times is by no means a trivial matter. For example, if we consider the simple case where the total Hamiltonian  $H$  is time-independent, we find from eq. (13.62) that

$$U_c(t, t') = \exp\{iH_c t\} \exp\{-iH(t - t')\} \exp\{-iH_c t'\} \quad (14.11)$$

and the limit of this expression for  $t$  or  $t' \rightarrow \pm\infty$  is undefined, because of its oscillatory character.

With these difficulties in mind, let us return to the physics of the situation. We shall ultimately be concerned with matrix elements of the transition operator. If, instead of (generalized) plane waves, the initial and final states

are taken to be *wave packets*, the undesirable transients introduced by the oscillations of  $U_c(t, t')$  can be shown to cancel out. Since the wave packet treatment is very lengthy and can be found in detail elsewhere [2], we shall indicate here two formal devices which do not require the use of wave packets.

We begin by discussing the limiting procedure of Gell-Mann and Goldberger [3]. It is defined by

$$\lim_{t \rightarrow -\infty} F(t) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t'} F(t') dt' \quad (14.12a)$$

and

$$\lim_{t \rightarrow +\infty} F(t) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-\varepsilon t'} F(t') dt'. \quad (14.12b)$$

Performing an integration by parts, we find that

$$\lim_{t \rightarrow -\infty} F(t) = \lim_{\varepsilon \rightarrow 0^+} \left\{ [F(t') e^{\varepsilon t'}]_{-\infty}^0 - \int_{-\infty}^0 \frac{dF}{dt'} e^{\varepsilon t'} dt' \right\} \quad (14.13a)$$

and

$$\lim_{t \rightarrow +\infty} F(t) = \lim_{\varepsilon \rightarrow 0^+} \left\{ -[F(t') e^{-\varepsilon t'}]_0^{\infty} + \int_0^{\infty} \frac{dF}{dt'} e^{-\varepsilon t'} dt' \right\}. \quad (14.13b)$$

Therefore, if  $F(t)$  has proper limits  $F(\pm\infty)$  at  $t = \pm\infty$ , we see that if we first let  $t \rightarrow -\infty$  in eq. (14.13a) [or  $t \rightarrow +\infty$  in eq. (14.13b)] and then take the limit  $\varepsilon \rightarrow 0^+$ , we have

$$\lim_{t \rightarrow -\infty} F(t) = F(-\infty); \quad \lim_{t \rightarrow +\infty} F(t) = F(+\infty). \quad (14.14)$$

On the contrary, if  $F(t)$  oscillates at large  $|t|$ , these oscillations will be damped by the exponential factors. For example,

$$\lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t} \sin t dt = - \lim_{\varepsilon \rightarrow 0^+} \frac{\alpha \varepsilon}{\alpha^2 + \varepsilon^2} = 0. \quad (14.15)$$

Let us now apply this limiting process to the evolution operators  $U_c(t, t')$ . We define the four operators

$$U_c(t, -\infty) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t'} U_c(t, t') dt', \quad (14.16a)$$

$$U_c(t, +\infty) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-\varepsilon t'} U_c(t, t') dt', \quad (14.16b)$$

$$U_c(-\infty, t) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t'} U_c(t', t) dt', \quad (14.16c)$$

$$U_c(+\infty, t) = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-\varepsilon t'} U_c(t', t) dt'. \quad (14.16d)$$

We note from eq. (14.16a) that the prescription we have adopted amounts to "feeding in" the incident beam over an infinite period of time. This is due to the fact that the incident beam is described by a monoenergetic plane wave [4].

It is a simple matter to show that the evolution operators (14.16) with one infinite argument satisfy the same integral equations as  $U_c(t, t')$ . For example

$$U_c(t, -\infty) = I - i \int_{-\infty}^t V_c(t') U_c(t', -\infty) dt'. \quad (14.17)$$

The group property (13.8) also holds when one of the arguments of the evolution operator is infinite. For example, from eq. (14.16a) we have

$$\begin{aligned} U_c(t, -\infty) &= \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t''} U_c(t, t'') dt'' \\ &= \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t''} U_c(t, t') U_c(t', t'') dt'' \\ &= U_c(t, t') U_c(t', -\infty). \end{aligned} \quad (14.18a)$$

Similarly, one also has

$$U_c(t, +\infty) = U_c(t, t') U_c(t', +\infty), \quad (14.18b)$$

$$U_c(+\infty, t) = U_c(+\infty, t') U_c(t', t) \quad (14.18c)$$

and

$$U_c(-\infty, t) = U_c(-\infty, t') U_c(t', t). \quad (14.18d)$$

We may also use eqs. (14.16a) and (13.57) to compute

$$\begin{aligned} U_c^\dagger(t, -\infty) &= \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t'} U_c^\dagger(t, t') dt' \\ &= \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t'} U_c(t', t) dt' \\ &= U_c(-\infty, t) \end{aligned} \quad (14.19a)$$

where the last line follows from the definition (14.16c). Similarly,

$$U_c^\dagger(t, +\infty) = U_c(+\infty, t), \quad (14.19b)$$

$$U_c^\dagger(+\infty, t) = U_c(t, +\infty) \quad (14.19c)$$

and

$$U_c^\dagger(-\infty, t) = U_c(t, -\infty). \quad (14.19d)$$

It is important to note that the relations (14.19) do not necessarily imply that the operators  $U_c$  with an infinite argument are unitary, since the corresponding inverse operators  $U_c^{-1}$  have not yet been defined.

Before we investigate this question, let us describe another limiting procedure, due to Sunakawa [5], which may be used to define the operators



$U_c$  with an infinite argument. It is obtained by extending eqs. (13.56) and (13.58) to read

$$U_c(t, \pm\infty) = I + i \lim_{\varepsilon \rightarrow 0^+} \int_t^{\pm\infty} e^{-\varepsilon|t'|} U_c(t, t') V_c(t') dt' \quad (14.20a)$$

and

$$U_c(\pm\infty, t) = I - i \lim_{\varepsilon \rightarrow 0^+} \int_t^{\pm\infty} e^{-\varepsilon|t'|} V_c(t') U_c(t', t) dt'. \quad (14.20b)$$

This device is related to the *adiabatic switching* of the interaction, which consists in replacing  $V_c(t)$  by  $V_c^{\text{ad}}(t) = \exp[-\varepsilon|t|]V_c(t)$  and was originally used by Lippmann and Schwinger [6]. Using the definitions (14.20) it is a simple matter to prove [5] that the operators  $U_c(t, \pm\infty)$  and  $U_c(\pm\infty, t)$  satisfy the important relations (14.18) and (14.19), as in the case of the Gell-Mann and Goldberger limiting procedure.

Let us now focus our attention on the operators  $U_c(0, \pm\infty)$  and  $U_c(\pm\infty, 0)$ . We begin by examining the simple case for which there is only *one* arrangement channel, i.e. one way of splitting the total Hamiltonian. We shall write

$$H = H_0 + V \quad (14.21)$$

and denote the eigenstates of  $H_0$  by the symbols  $\Phi_\alpha, \Phi_\beta, \dots$  where the indices  $\alpha, \beta, \dots$  refer to a collection of quantum numbers. We assume that  $H_0$  has no bound states. We then define for this case the Møller (wave) operators [7–10]

$$\Omega^{(\pm)} = U(0, \mp\infty) \quad (14.22)$$

and

$$\Omega^{(\pm)\dagger} = U(\mp\infty, 0). \quad (14.23)$$

We see that the operators  $\Omega^{(\pm)}$  convert an eigenstate  $\Phi_\alpha$  of the “reference problem” (governed by the Hamiltonian  $H_0$ ) into the corresponding (continuum) eigenstate  $\Psi_\alpha$  of the full Hamiltonian (at the time  $t = 0$ ) [11]. Thus

$$\Psi_\alpha^{(\pm)} = \Omega^{(\pm)}\Phi_\alpha. \quad (14.24)$$

In terms of Dirac’s bra and ket notation we may also write eq. (14.24) as [12]

$$|\Psi_\alpha^{(\pm)}\rangle = \Omega^{(\pm)}|\Phi_\alpha\rangle \quad (14.25)$$

and

$$\langle\Psi_\alpha^{(\pm)}| = \langle\Phi_\alpha|\Omega^{(\pm)\dagger}. \quad (14.26)$$

We note from the above equations that the matrix elements of the Møller operators between free states are given by

$$\langle\Phi_\beta|\Omega^{(\pm)}|\Phi_\alpha\rangle = \langle\Phi_\beta|\Psi_\alpha^{(\pm)}\rangle \quad (14.27)$$

and

$$\langle\Phi_\beta|\Omega^{(\pm)\dagger}|\Phi_\alpha\rangle = \langle\Psi_\beta^{(\pm)}|\Phi_\alpha\rangle. \quad (14.28)$$

Let us now study some properties of the Møller operators. First of all, since [13]

$$\langle\Phi_\beta|\Phi_\alpha\rangle = \delta_{\beta\alpha} \quad (14.29)$$

we deduce from eq. (14.25) that

$$\Omega^{(\pm)} = \sum_{\alpha} |\Psi_{\alpha}^{(\pm)}\rangle \langle \Phi_{\alpha}|. \quad (14.30)$$

Moreover, upon using eqs. (14.11), (14.16) and (14.22) we obtain an "explicit" form of  $\Omega^{(\pm)}$ , namely

$$\begin{aligned} \Omega^{(\pm)} &= \lim_{t \rightarrow \mp \infty} U(0, t) \\ &= \lim_{t \rightarrow \mp \infty} \exp(iHt) \exp(-iH_0t) \\ &= \lim_{\varepsilon \rightarrow 0^+} \mp \varepsilon \int_0^{\mp \infty} \exp(\pm \varepsilon t) \exp(iHt) \exp(-iH_0t) dt. \end{aligned} \quad (14.31)$$

If we assume that the states  $\Phi_{\alpha}$  form a complete set and insert in eq. (14.31) the completeness relation

$$\sum_{\alpha} |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}| = I \quad (14.32)$$

we find that

$$\Omega^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \mp \varepsilon \sum_{\alpha} \int_0^{\mp \infty} \exp(\pm \varepsilon t) \exp(iHt) |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}| \exp(-iH_0t) dt \quad (14.33)$$

or

$$\Omega^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \mp \varepsilon \sum_{\alpha} \int_0^{\mp \infty} \exp(\pm \varepsilon t) \exp(iHt) |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}| \exp(-iE_{\alpha}t) dt. \quad (14.34)$$

Performing the integration, we obtain

$$\Omega^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \sum_{\alpha} \frac{\pm i\varepsilon}{E_{\alpha} - H \pm i\varepsilon} |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}|. \quad (14.35)$$

Upon comparison of eqs. (14.30) and (14.35) we see that [14]

$$\Psi_{\alpha}^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{\pm i\varepsilon}{E_{\alpha} - H \pm i\varepsilon} \Phi_{\alpha}. \quad (14.36)$$

We now examine the question of the *unitarity* of the Møller operators. To this end, we first observe that

$$\langle \Psi_{\beta}^{(\pm)} | \Psi_{\alpha}^{(\pm)} \rangle = \delta_{\beta\alpha} \quad (14.37)$$

since the solutions of the full problem corresponding to a given type of boundary condition are orthonormal. We then have from eqs. (14.25) and (14.26)

$$\Omega^{(\pm)\dagger} \Omega^{(\pm)} = \sum_{\alpha} \sum_{\beta} |\Phi_{\beta}\rangle \langle \Psi_{\beta}^{\pm} | \Psi_{\alpha}^{\pm} \rangle \langle \Phi_{\alpha}| = \sum_{\alpha} |\Phi_{\alpha}\rangle \langle \Phi_{\alpha}|.$$

Upon using the completeness relation (14.32) for the states  $\Phi_{\alpha}$ , we then find that

$$\Omega^{(\pm)\dagger} \Omega^{(\pm)} = I. \quad (14.38)$$

Therefore the Møller operators  $\Omega^{(\pm)}$  are *isometric*, i.e. they do not change the length of a vector. Indeed,

$$\langle \Omega^{(\pm)} \Psi | \Omega^{(\pm)} \Psi \rangle = \langle \Psi | \Omega^{(\pm)\dagger} \Omega^{(\pm)} \Psi \rangle = \langle \Psi | \Psi \rangle. \quad (14.39)$$

On the other hand, we also have

$$\Omega^{(\pm)} \Omega^{(\pm)\dagger} = \sum_{\alpha} \sum_{\beta} |\Psi_{\beta}^{(\pm)}\rangle \langle \Phi_{\beta} | \Phi_{\alpha}\rangle \langle \Psi_{\alpha}^{(\pm)}| = \sum_{\alpha} |\Psi_{\alpha}^{(\pm)}\rangle \langle \Psi_{\alpha}^{(\pm)}| \quad (14.40)$$

where we have used eq. (14.29). Let us denote by  $\Psi^{(B)}$  the state vectors corresponding to the possible bound states of the total Hamiltonian  $H$ . From the completeness relation

$$\sum_{\alpha} |\Psi_{\alpha}^{(\pm)}\rangle \langle \Psi_{\alpha}^{(\pm)}| + \sum_B |\Psi^{(B)}\rangle \langle \Psi^{(B)}| = I \quad (14.41)$$

we deduce that

$$\Omega^{(\pm)} \Omega^{(\pm)\dagger} = I - A \quad (14.42)$$

where

$$A = \sum_B |\Psi^{(B)}\rangle \langle \Psi^{(B)}| \quad (14.43)$$

is the projection operator onto the bound states of  $H$ . Hence, from eqs. (14.38) and (14.42) we infer that the Møller operators  $\Omega^{(\pm)}$  are unitary only if the Hamiltonians  $H$  and  $H_0$  have no bound states. This result is in contrast with the unitarity property of the evolution operator  $U(t, t')$  for finite arguments.

Next, we remark that

$$E_{\alpha} \Psi_{\alpha}^{(\pm)} = H \Psi_{\alpha}^{(\pm)} = H \Omega^{(\pm)} \Phi_{\alpha} \quad (14.44a)$$

and also

$$E_{\alpha} \Psi_{\alpha}^{(\pm)} = \Omega^{(\pm)} E_{\alpha} \Phi_{\alpha} = \Omega^{(\pm)} H_0 \Phi_{\alpha}. \quad (14.44b)$$

Therefore, since the states  $\Phi_{\alpha}$  form a complete set, we have

$$H \Omega^{(\pm)} = \Omega^{(\pm)} H_0. \quad (14.45)$$

Moreover, upon using the fact that  $H$  and  $H_0$  are Hermitian operators, we also find that

$$\Omega^{(\pm)\dagger} H = H_0 \Omega^{(\pm)\dagger}. \quad (14.46)$$

Hence, if  $\Psi$  is an eigenstate of  $H$  corresponding to the energy  $E$ , we may write

$$H_0 \Omega^{(\pm)\dagger} \Psi = E \Omega^{(\pm)\dagger} \Psi. \quad (14.47)$$

In particular, if the energy  $E$  lies in the spectrum of  $H$  but not in that of  $H_0$  (i.e. corresponds to a bound state  $\Psi^{(B)}$ ) we must have

$$\Omega^{(\pm)\dagger} |\Psi^{(B)}\rangle = 0 \quad (14.48)$$

so that the operators  $\Omega^{(\pm)\dagger}$  annihilate the bound states  $\Psi^{(B)}$ . This property evidently implies that

$$\Omega^{(\pm)\dagger} A = 0 \quad (14.49)$$

where  $A$  is given by eq. (14.43).

We now generalize the foregoing discussion to the case where the total Hamiltonian  $H$  may be split in various arrangement channels according to eq. (14.1). To this end, let us first introduce the channel projection operator

$$A_c = \sum_{\gamma} |\Phi_{c,\gamma}\rangle \langle \Phi_{c,\gamma}| \quad (14.50)$$

where the index  $\gamma$  summarizes a collection of quantum numbers and the summation runs over the set of states  $\Phi_{c,\gamma}$  belonging to the arrangement channel  $c$ . (We recall that in general the channel states  $\Phi_{c,\gamma}$  do not form a complete set.) We shall call  $\mathcal{R}_c$  the “channel space” containing the states  $\Phi_n \equiv \Phi_{c,\gamma}$  appearing in the sum (14.50). We then define the Møller wave operators as

$$\Omega_c^{(\pm)} = U_c(0, \mp\infty) A_c \quad (14.51)$$

and we note that

$$\Omega_c^{(\pm)\dagger} = A_c U_c(\mp\infty, 0) \quad (14.52)$$

since  $A_c^\dagger = A_c$  and  $U_c^\dagger(0, \mp\infty) = U_c(\mp\infty, 0)$ . We emphasize that the operators  $\Omega_c^{(\pm)}$  act only on the channel space  $\mathcal{R}_c$ . Thus, if we consider only those states  $\Phi_n \equiv \Phi_{c,\gamma}$  appearing in eq. (14.50) we may write the eigenstates  $\Psi_n^{(\pm)}$  of the full Hamiltonian (at the time  $t = 0$ ) originating from  $\Phi_n$  as

$$\Psi_n^{(\pm)} = \Omega_c^{(\pm)} \Phi_n. \quad (14.53a)$$

In particular, we have in the initial and final arrangement channels [with  $a \equiv (i, \alpha)$  and  $b \equiv (f, \beta)$ ]

$$\Psi_a^{(\pm)} = \Omega_i^{(\pm)} \Phi_a \quad (14.53b)$$

and

$$\Psi_b^{(\pm)} = \Omega_f^{(\pm)} \Phi_b. \quad (14.53c)$$

Similarly,

$$\langle \Psi_n^{(\pm)} | = \langle \Phi_n | \Omega_c^{(\pm)\dagger}, \quad (14.54a)$$

$$\langle \Psi_a^{(\pm)} | = \langle \Phi_a | \Omega_i^{(\pm)\dagger} \quad (14.54b)$$

and

$$\langle \Psi_b^{(\pm)} | = \langle \Phi_b | \Omega_f^{(\pm)\dagger}. \quad (14.54c)$$

According to eqs. (14.11), (14.16) and (14.51) we also have

$$\begin{aligned} \Omega_c^{(\pm)} &= \lim_{t \rightarrow \mp\infty} U_c(0, t) A_c = \lim_{t \rightarrow \mp\infty} \exp(iHt) \exp(-iH_c t) A_c \\ &= \lim_{\varepsilon \rightarrow 0^+} \mp \varepsilon \int_0^{\mp\infty} \exp(\pm \varepsilon t) \exp(iHt) \exp(-iH_c t) dt A_c. \end{aligned} \quad (14.55)$$

Since the Møller operators  $\Omega_c^{(\pm)}$  only act on the channel space  $\mathcal{R}_c$ , we may generalize eq. (14.38) by writing

$$\Omega_c^{(\pm)\dagger} \Omega_c^{(\pm)} = A_c \quad (14.56)$$

so that the  $\Omega_c^{(\pm)}$  are *partially isometric* (from  $\mathcal{R}_c$ ).

Let us investigate the relationships between Møller operators belonging to different arrangement channels. We begin by noting that for two arrangement channels  $c$  and  $c'$  corresponding to *different* channel Hamiltonians  $H_c$  and  $H_{c'}$  one has

$$\langle \Phi_n | \Phi_n \rangle = \langle \Phi_{c',\gamma'} | \Phi_{c,\gamma} \rangle \neq 0. \quad (14.57a)$$

In particular, if the initial and final “free” states  $\Phi_a$  and  $\Phi_b$  belong to different arrangement channels (i.e. are eigenstates of two different channel Hamiltonians  $H_i$  and  $H_f$ ), one has

$$\langle \Phi_b | \Phi_a \rangle = \langle \Phi_{i,\alpha} | \Phi_{f,\beta} \rangle \neq 0. \quad (14.57b)$$

This is in contrast with the “one arrangement channel” situation for which eq. (14.29) holds. Hence in general the channel projection operators  $A_c$  and  $A_{c'}$  are such that

$$A_c A_{c'} \neq 0. \quad (14.58)$$

On the other hand, eq. (14.37) may be generalized to the multi-channel case to read

$$\langle \Psi_b^{(\pm)} | \Psi_a^{(\pm)} \rangle = \delta_{ba}. \quad (14.59)$$

This relation expresses the fact that no matter how we solve the full problem we get the same orthonormal set of solutions even though the solutions of the reference problem are not orthogonal. In particular, the full states that develop from (or into) one arrangement channel are orthogonal to those corresponding to another one. A rigorous proof of eq. (14.59) is very involved and will not be given here. It may be found in the references [15] and [16] listed at the end of this chapter.

Let us now return to the Møller operators. From eqs. (14.51), (14.52), (14.56) and (14.59) we see that

$$\Omega_c^{(\pm)\dagger} \Omega_c^{(\pm)} = A_c \delta_{c,c} \quad (14.60)$$

which is the generalization of eq. (14.38).

In order to generalize eq. (14.42), we first note that because of the relation (14.59) the spaces of all eigenstates  $\Psi_n^{(\pm)}$  of the full Hamiltonian which develop from (or into) the arrangement channel  $c$  are mutually orthogonal. Moreover, if we call  $Q_c^{(\pm)}$  a projection operator into one of these spaces, we have

$$\Omega_c^{(\pm)} \Omega_c^{(\pm)\dagger} = Q_c^{(\pm)}. \quad (14.61)$$

Since all the eigenstates of the full Hamiltonian (except the genuine bound states  $\Psi^{(B)}$  such that *all* the particles are bound) must be decomposable into states that develop from (or into) one of the arrangement channels, we have the (generalized) completeness relation

$$\sum_c \Omega_c^{(\pm)} \Omega_c^{(\pm)\dagger} = I - A \quad (14.62)$$

where  $\Lambda$  is the bound state projection operator (14.43). This sum contains *all* the arrangement channels, including the one in which all the “elementary” particles participating in the collision are free.

We may also generalize eq. (14.45). Indeed, from the Schrödinger equations  $H\Psi_n^{(\pm)} = E_n\Psi_n^{(\pm)}$  and  $H_c\Phi_n = E_n\Phi_n$  we deduce that

$$H\Omega_c^{(\pm)} = \Omega_c^{(\pm)}H_c \quad (14.63)$$

from which we may also infer that the operators  $\Omega_c^{(\pm)\dagger}$  annihilate the bound states of  $H$  [see the discussion following eq. (14.45)]. Hence

$$\Omega_c^{(\pm)\dagger}\Lambda = 0. \quad (14.64)$$

Finally, we can use eqs. (14.53) and (14.55) to generalize eq. (14.36). This yields

$$\Psi_n^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{\pm i\varepsilon}{E_n - H \pm i\varepsilon} \Phi_n. \quad (14.65)$$

Since  $H_c\Phi_n = E_n\Phi_n$  and  $H = H_c + V_c$  we may also write this result as

$$\Psi_n^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_n - H \pm i\varepsilon} (E_n - H_c - V_c + V_c \pm i\varepsilon) \Phi_n$$

or

$$\Psi_n^{(\pm)} = \Phi_n + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_n - H \pm i\varepsilon} V_c \Phi_n. \quad (14.66a)$$

In particular, we have in the initial and final arrangement channels

$$\Psi_a^{(\pm)} = \Phi_a + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_a - H \pm i\varepsilon} V_i \Phi_a \quad (14.66b)$$

and

$$\Psi_b^{(\pm)} = \Phi_b + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_b - H \pm i\varepsilon} V_f \Phi_b. \quad (14.66c)$$

Using the hermiticity property of the operators  $H$  and  $V_c$ , we also find that

$$\langle \Psi_n^{(\pm)} | = \langle \Phi_n | + \lim_{\varepsilon \rightarrow 0^+} \langle \Phi_n | V_c \frac{1}{E_n - H \mp i\varepsilon}, \quad (14.67a)$$

$$\langle \Psi_a^{(\pm)} | = \langle \Phi_a | + \lim_{\varepsilon \rightarrow 0^+} \langle \Phi_a | V_i \frac{1}{E_a - H \mp i\varepsilon} \quad (14.67b)$$

and

$$\langle \Psi_b^{(\pm)} | = \langle \Phi_b | + \lim_{\varepsilon \rightarrow 0^+} \langle \Phi_b | V_f \frac{1}{E_b - H \mp i\varepsilon}. \quad (14.67c)$$

The equations (14.66)–(14.67) are of fundamental importance and will be frequently used below.

## 14.2. The $S$ matrix

Having studied the evolution operators having one infinite time argument, we are now ready to define a *collision operator* or *collision matrix* [17] which relates the state vectors describing the system in the remote past ( $t' \rightarrow -\infty$ ) and in the far future ( $t \rightarrow +\infty$ ).

We begin by considering the simple case for which there is only *one* arrangement channel, so that the total Hamiltonian  $H$  is decomposed according to eq. (14.21) into  $H_0$  (the asymptotic Hamiltonian) and  $V$  (the interaction between the colliding particles). We then define the collision operator  $S$  as the composition of two Møller operators, namely

$$S = U(+\infty, 0)U(0, -\infty) = \Omega^{(-)\dagger}\Omega^{(+)} \quad (14.68)$$

We assume that this operator acts on the eigenstates  $\Phi_\alpha, \Phi_\beta, \dots$  of  $H_0$  (i.e. asymptotic “free” states having respectively the set of quantum numbers summarized by  $\alpha, \beta, \dots$ ).

Let us calculate the matrix elements of the operator  $S$  between two “asymptotic” states  $\Phi_\alpha$  and  $\Phi_\beta$ . We obtain in this way the *S-matrix elements*

$$\langle \beta | S | \alpha \rangle \equiv \langle \Phi_\beta | S | \Phi_\alpha \rangle = \langle \Phi_\beta | \Omega^{(-)\dagger} \Omega^{(+)} | \Phi_\alpha \rangle \quad (14.69)$$

or

$$\langle \beta | S | \alpha \rangle = \langle \Psi_\beta^{(-)} | \Psi_\alpha^{(+)} \rangle \quad (14.70)$$

where we have used eq. (14.25) and also eq. (14.26) (in which we have replaced  $\alpha$  by  $\beta$ ). We note from eq. (14.70) that the  $S$ -matrix elements are *time-independent*. In fact, the expression (14.70) coincides with that of the  $S$ -matrix elements in the time-independent formal scattering theory [18]. We also remark from eq. (14.70) that the  $S$ -matrix element  $\langle \beta | S | \alpha \rangle$  represents the probability amplitude of finding the system (described in the interaction picture by the state vector  $\Psi_\alpha^{(+)}$ ) into the state  $\Psi_\beta^{(-)}$ . We recall that the state  $\Psi_\alpha^{(+)}$  originates from the “free” state  $\Phi_\alpha$  while the state  $\Psi_\beta^{(-)}$  goes over to  $\Phi_\beta$ . We note, however, that the representation (14.70) of the  $S$ -matrix element does not make any reference to the splitting of the total Hamiltonian  $H$  into an “unperturbed” part  $H_0$  and a “perturbation”  $V$ .

We shall now prove that the  $S$ -operator (14.68), defined over the set of states  $\Phi_\alpha$  (which we assume to be complete) is *unitary*. Indeed, one has

$$\begin{aligned} S^\dagger S &= \Omega^{(+)\dagger} \Omega^{(-)} \Omega^{(-)\dagger} \Omega^{(+)} \\ &= \Omega^{(+)\dagger} (1 - A) \Omega^{(+)} = \Omega^{(+)\dagger} \Omega^{(+)} = I \end{aligned} \quad (14.71a)$$

where we have used successively eqs. (14.42), (14.49) and (14.38). Similarly,

$$\begin{aligned} SS^\dagger &= \Omega^{(-)\dagger} \Omega^{(+)} \Omega^{(+)\dagger} \Omega^{(-)} \\ &= \Omega^{(-)\dagger} (1 - A) \Omega^{(-)} = \Omega^{(-)\dagger} \Omega^{(-)} = I. \end{aligned} \quad (14.71b)$$

Therefore

$$S^\dagger S = SS^\dagger = I. \quad (14.72)$$

We may also obtain this result by using  $S$ -matrix elements. Thus we write

$$\begin{aligned}\langle\beta|S^\dagger S|\alpha\rangle &= \sum_\gamma \langle\beta|S^\dagger|\gamma\rangle\langle\gamma|S|\alpha\rangle \\ &= \sum_\gamma \langle\Psi_\beta^{(+)}|\Psi_\gamma^{(-)}\rangle\langle\Psi_\gamma^{(-)}|\Psi_\alpha^{(+)}\rangle\end{aligned}\quad (14.73)$$

where we have used eq. (14.70). With the help of eqs. (14.41) and (14.43), we obtain

$$\langle\beta|S^\dagger S|\alpha\rangle = \langle\Psi_\beta^{(+)}|I - A|\Psi_\alpha^{(+)}\rangle. \quad (14.74)$$

Moreover, since the bound state wave functions  $\Psi^{(B)}$  appearing in  $A$  are orthogonal to the continuum wave functions  $\Psi^{(\pm)}$  and because the continuum wave functions satisfy eq. (14.37), we have

$$\langle\beta|S^\dagger S|\alpha\rangle = \sum_\gamma \langle\beta|S^\dagger|\gamma\rangle\langle\gamma|S|\alpha\rangle = \delta_{\beta\alpha}. \quad (14.75a)$$

Similarly,

$$\langle\beta|SS^\dagger|\alpha\rangle = \sum_\gamma \langle\beta|S|\gamma\rangle\langle\gamma|S^\dagger|\alpha\rangle = \delta_{\beta\alpha} \quad (14.75b)$$

which proves the unitarity of the  $S$ -matrix. We note that the completeness relations (14.32) and (14.41) which express the content of the *superposition principle* and of the *conservation of probability*, induce the important properties (14.38) and (14.42) of the Møller operators and therefore the unitarity of the  $S$ -operator (or  $S$ -matrix).

Another interesting property of the  $S$ -operator (14.68) follows from the relations (14.45) and (14.46) satisfied by the Møller operators. That is,

$$\Omega^{(-)\dagger}H\Omega^{(+)} = \Omega^{(-)\dagger}\Omega^{(+)}H_0 = H_0\Omega^{(-)\dagger}\Omega^{(+)} \quad (14.76)$$

so that

$$[S, H_0] = 0. \quad (14.77)$$

The operator

$$S' = \Omega^{(+)}\Omega^{(-)\dagger} \quad (14.78)$$

is also sometimes referred to as the  $S$ -matrix or  $S$ -operator. We note from eqs. (14.38) and (14.42) that

$$S'^\dagger S' = S' S'^\dagger = I - A. \quad (14.79)$$

Moreover, from eqs. (14.45) and (14.46), we have

$$\Omega^{(+)}\Omega^{(-)\dagger}H = \Omega^{(+)}H_0\Omega^{(-)\dagger} = H\Omega^{(+)}\Omega^{(-)\dagger} \quad (14.80)$$

and therefore

$$[S', H] = 0. \quad (14.81)$$

Furthermore, if the  $\Psi_\alpha^{(\pm)}$  are a complete set spanning the continuous spectrum of  $H$  (i.e. excluding the bound states  $\Psi^{(B)}$ ) we see that

$$\langle\Psi_\beta^{(\pm)}|S'|\Psi_\alpha^{(\pm)}\rangle = \langle\Psi_\beta^{(-)}|\Psi_\alpha^{(+)}\rangle = \langle\Phi_\beta|S|\Phi_\alpha\rangle. \quad (14.82)$$



Thus the matrix elements of  $S'$  computed on the basis of the scattering states  $\Psi^{(\pm)}$  are the same as those of  $S$  evaluated between the corresponding reference states  $\Phi$ .

Let us generalize our discussion to the case where there is more than one arrangement channel [19]. Instead of one  $S$ -operator we now have a *set* of  $S$ -operators

$$S_{c'c} = \Omega_c^{(-)\dagger} \Omega_c^{(+)} \quad (14.83a)$$

Using a notation which refers more explicitly to the initial and final arrangement channels of a collision process, we shall also write

$$S_{fi} = \Omega_f^{(-)\dagger} \Omega_i^{(+)} \quad (14.83b)$$

The “ $S$ -matrix elements” are obtained by evaluating the above  $S$ -operators between asymptotic states which are respectively eigenstates of the initial and final channel Hamiltonians. That is

$$\langle b|S|a \rangle \equiv \langle f\beta|S_{fi}|i\alpha \rangle = \langle \Phi_{f,\beta}|S_{fi}|\Phi_{i,\alpha} \rangle = \langle \Phi_b|S_{fi}|\Phi_a \rangle. \quad (14.84)$$

Hence

$$\langle b|S|a \rangle = \langle \Phi_b|\Omega_f^{(-)\dagger} \Omega_i^{(+)}|\Phi_a \rangle = \langle \Psi_b^{(-)}|\Psi_a^{(+)} \rangle. \quad (14.85)$$

This result generalizes the formula (14.70) which we obtained in the “one arrangement channel” situation.

Let us now return to the operators  $S_{c'c}$  defined by eq. (14.83a). Using successively eqs. (14.62), (14.64) and (14.60), we find that

$$\begin{aligned} \sum_c S_{f'c} S_{fc}^\dagger &= \sum_c \Omega_{f'}^{(-)\dagger} \Omega_c^{(+)} \Omega_c^{(+)\dagger} \Omega_f^{(-)} \\ &= \Omega_{f'}^{(-)\dagger} (1 - A) \Omega_f^{(-)} = \Omega_{f'}^{(-)\dagger} \Omega_f^{(-)} = A_{f'} \delta_{f'f}. \end{aligned} \quad (14.86a)$$

Similarly,

$$\sum_c S_{ci}^\dagger S_{ci} = A_i \delta_{ii}. \quad (14.86b)$$

These equations imply the *unitarity* of the general (multi-channel)  $S$ -matrix. Indeed, we have

$$\begin{aligned} \sum_c \langle b|S_{ci}^\dagger S_{ci}|a \rangle &= \sum_c \sum_\gamma \langle \Phi_{f,\beta}|S_{ci}^\dagger|\Phi_{c,\gamma}^\dagger \rangle \langle \Phi_{c,\gamma}^\dagger|S_{ci}|\Phi_{i,\alpha} \rangle \\ &= \sum_c \sum_\gamma \langle \Phi_{f,\beta}|S_{ci}^\dagger|\Phi_{c,\gamma}^\dagger \rangle \langle \Phi_{c,\gamma}|S_{ci}|\Phi_{i,\alpha} \rangle \\ &= \sum_{n \equiv (c,\gamma)} \langle b|S_{ci}^\dagger|n \rangle \langle n|S_{ci}|a \rangle = \delta_{ba}. \end{aligned} \quad (14.87a)$$

In obtaining this result we have inserted a complete set of states  $\Phi_c^\dagger$ , used the fact that the Møller operators contain projection operators  $A_c$  acting on channel states, and also made use of eq. (14.86b). Similarly, one also has

$$\sum_c \langle b|S_{f'c} S_{fc}^\dagger|a \rangle = \sum_n \langle b|S_{f'c}|n \rangle \langle n|S_{fc}^\dagger|a \rangle = \delta_{ba}. \quad (14.87b)$$

We note that these relations are considerably more complicated than the simple, "one arrangement channel" unitarity relations (14.75). To simplify the notation we shall write below the unitarity relations (for both cases of one or more than one arrangement channels) in the form

$$\sum_n \langle b|S^\dagger|n\rangle\langle n|S|a\rangle = \delta_{ba} \quad (14.87c)$$

and

$$\sum_n \langle b|S|n\rangle\langle n|S^\dagger|a\rangle = \delta_{ba}. \quad (14.87d)$$

Another interesting property of the  $S_{fi}$  operators (14.83) follows from the fact that the channel Møller operators satisfy eq. (14.63). Thus we have for example

$$\Omega_i^{(+)}H_i = H\Omega_i^{(+)}. \quad (14.88)$$

Multiplying on the left by  $\Omega_f^{(-)\dagger}$ , we find that

$$\begin{aligned} \Omega_f^{(-)\dagger}\Omega_i^{(+)}H_i &= \Omega_f^{(-)\dagger}H\Omega_i^{(+)} \\ &= H_f\Omega_f^{(-)\dagger}\Omega_i^{(+)} \end{aligned} \quad (14.89)$$

or, using eq. (14.83b),

$$S_{fi}H_i = H_fS_{fi}. \quad (14.90)$$

In the particular case where there is only one arrangement channel (so that  $H_i = H_f$ ), eq. (14.90) yields the result (14.77) proved above.

Let us now obtain a more explicit expression for the  $S$ -matrix elements. We start from the representation (14.85), which we rewrite as

$$\begin{aligned} \langle b|S|a\rangle &= \langle \Psi_b^{(-)}|\Psi_a^{(+)}\rangle \\ &= \langle \Psi_b^{(+)}|\Psi_a^{(+)}\rangle + \langle \Psi_b^{(-)} - \Psi_b^{(+)}|\Psi_a^{(+)}\rangle \end{aligned} \quad (14.91)$$

or, by using eq. (14.59),

$$\langle b|S|a\rangle = \delta_{ba} + \langle \Psi_b^{(-)} - \Psi_b^{(+)}|\Psi_a^{(+)}\rangle. \quad (14.92)$$

Taking into account eq. (14.67c), we may transform the right-hand side of this equation as

$$\begin{aligned} \langle b|S|a\rangle &= \delta_{ba} + \lim_{\varepsilon \rightarrow 0^+} \left\langle \Phi_b \left| V_f \left( \frac{1}{E_b - H + i\varepsilon} - \frac{1}{E_b - H - i\varepsilon} \right) \right| \Psi_a^{(+)} \right\rangle \\ &= \delta_{ba} + \lim_{\varepsilon \rightarrow 0^+} \left( \frac{1}{E_b - E_a + i\varepsilon} - \frac{1}{E_b - E_a - i\varepsilon} \right) \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle \\ &= \delta_{ba} - \lim_{\varepsilon \rightarrow 0^+} \frac{2i\varepsilon}{(E_b - E_a)^2 + \varepsilon^2} \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle. \end{aligned} \quad (14.93)$$

Consider now the expression

$$\lim_{\varepsilon \rightarrow 0^+} \frac{\varepsilon}{(E_b - E_a)^2 + \varepsilon^2}. \quad (14.94)$$

This quantity obviously vanishes for  $E_a \neq E_b$ , while it is infinite for  $E_a = E_b$ . Thus

$$\lim_{\varepsilon \rightarrow 0^+} \frac{\varepsilon}{(E_b - E_a)^2 + \varepsilon^2} = C\delta(E_a - E_b) \quad (14.95)$$

where  $C$  is a constant. One easily shows that  $C = \pi$  [20] so that

$$\langle b|S|a \rangle = \delta_{ba} - 2\pi i\delta(E_a - E_b)\langle \Phi_b|V_f|\Psi_a^{(+)} \rangle. \quad (14.96)$$

In a completely similar way, one can prove that

$$\langle b|S|a \rangle = \langle \Psi_b^{(-)}|\Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)}|\Psi_a^{(-)} \rangle + \langle \Psi_b^{(-)}|\Psi_a^{(+)} - \Psi_a^{(-)} \rangle$$

or

$$\langle b|S|a \rangle = \delta_{ba} - 2\pi i\delta(E_a - E_b)\langle \Psi_b^{(-)}|V_i|\Phi_a \rangle. \quad (14.97)$$

The comparison of eqs. (14.96) and (14.97) implies that *on the energy shell* ( $E_a = E_b$ ) one has

$$\langle \Phi_b|V_f|\Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)}|V_i|\Phi_a \rangle. \quad (14.98)$$

Indeed, for  $E_a \neq E_b$  the second term on the right-hand side of eqs. (14.96)–(14.97) vanishes independently of the value of the matrix elements  $\langle \Phi_b|V_f|\Psi_a^{(+)} \rangle$  or  $\langle \Psi_b^{(-)}|V_i|\Phi_a \rangle$ . On the contrary, for  $E_a = E_b$  the equality of the two expressions (14.96) and (14.97) of the  $S$ -matrix elements requires that eq. (14.98) must hold. The fact that  $\delta(E_a - E_b)$  is actually *infinite* for  $E_a = E_b$  should be no cause of alarm, since we shall eventually consider transitions into a group of states in the continuum centered about  $E = E_a = E_b$ .

It is also worth noting the difference between the symbol  $\delta_{ba}$  and  $\delta(E_a - E_b)$  in eqs. (14.96) and (14.97). The former strictly vanishes as soon as  $a \neq b$ , so that it disappears for transitions between different states. Only for pure elastic scattering in the forward direction is this term present. The latter delta function ensures *energy conservation* in a transition  $a \rightarrow b$ .

Until now we have studied the  $S$ -matrix within the framework of the *interaction picture*. It is important, however, to analyze the  $S$ -matrix from the point of view of the *Schrödinger* or the *Heisenberg* pictures. We shall do this for the simple case where there is only one arrangement channel, with  $H = H_0 + V$ .

Let us begin with the Schrödinger picture. In this case the “unperturbed” system prior to scattering is described by the state vector

$$\phi_\alpha(t) = \exp(-iH_0t)\Phi_\alpha = \exp(-iE_\alpha t)\Phi_\alpha \quad (14.99)$$

where  $\Phi_\alpha$  is the interaction picture eigenstate of  $H_0$  corresponding to the quantum numbers  $\alpha$ . The Schrödinger state function  $\Psi_s(t)$  for the complete system which at  $t = t_0$  reduces to  $\phi_\alpha(t_0)$  is given by

$$\Psi_s(t) = \exp\{-iH(t - t_0)\}\phi_\alpha(t_0). \quad (14.100)$$

The probability amplitude for finding the system at time  $t$  in the state

$$\phi_\beta(t) = \exp(-iH_0 t)\Phi_\beta = \exp(-iE_\beta t)\Phi_\beta \quad (14.101)$$

is therefore given by

$$\begin{aligned} & \langle \exp\{-iH_0 t\}\Phi_\beta | \exp\{-iH(t-t_0)\} | \exp\{-iH_0 t_0\}\Phi_\alpha \rangle \\ & = \langle \Phi_\beta | \exp\{iH_0 t\} \exp\{-iH(t-t_0)\} \exp\{-iH_0 t_0\} | \Phi_\alpha \rangle. \end{aligned} \quad (14.102)$$

Upon taking the limit of this expression for  $t_0 \rightarrow -\infty$  and  $t \rightarrow +\infty$  and using the limiting procedures defined in Section 14.1 we find that the probability amplitude (14.102) reduces to

$$\langle \Phi_\beta | \Omega^{(-)\dagger} \Omega^{(+)} | \Phi_\alpha \rangle = \langle \Psi_\beta^{(-)} | \Psi_\alpha^{(+)} \rangle = \langle \beta | S | \alpha \rangle \quad (14.103)$$

in accordance with eq. (14.70).

We now turn to the Heisenberg picture, in which the state vectors are independent of time while the dynamical variables are time-dependent. The scattering question is then: "What is the probability amplitude of finding the system in the far future in an eigenstate  $|\beta\rangle$  of the operator  $B(t = +\infty)$  when it was in the remote past in the eigenstate  $|\alpha\rangle$  of the operator  $A(t = -\infty)$ ?" The discussion following eq. (13.40) provides the answer to this question: the relevant transition amplitude is again given by eq. (14.102) or equivalently, by the  $S$ -matrix elements (14.103).

Further insight into this problem may be gained in the following way. Let us continue to assume that the simple decomposition  $H = H_0 + V$  holds. For the sake of simplicity we shall also suppose that neither  $H_0$  nor  $H$  has bound states. We define the Heisenberg operators [21]:

$$\Omega_H^{(\pm)}(t) = e^{iHt} \Omega_s^{(\pm)} e^{-iHt} \quad (14.104)$$

where  $\Omega_s^{(\pm)}$  are the Møller operators in the Schrödinger picture, and we assume that the Schrödinger, Heisenberg and interaction pictures coincide at  $t_0 = 0$ . Let  $A_H(t)$  be an operator in the Heisenberg picture which has no intrinsic time-dependence. It is convenient to introduce the in- and out-operators

$$A_H^{\text{in}}(t) = \Omega_H^{(+)}(t) A_H(t) \Omega_H^{(+)\dagger}(t) \quad (14.105a)$$

and

$$A_H^{\text{out}}(t) = \Omega_H^{(-)}(t) A_H(t) \Omega_H^{(-)\dagger}(t) \quad (14.105b)$$

which may be easily shown to satisfy the Heisenberg equations of motion

$$i \frac{d}{dt} A_H^{\text{in}}(t) = [A_H^{\text{in}}, H] \quad (14.106a)$$

and

$$i \frac{d}{dt} A_H^{\text{out}}(t) = [A_H^{\text{out}}, H] \quad (14.106b)$$

where the complete Hamiltonian  $H$  is evidently the same in the Schrödinger and Heisenberg pictures. These equations must be solved subject to the initial conditions

$$\lim_{t \rightarrow -\infty} A_H^{\text{in}}(t) = \lim_{t \rightarrow -\infty} A_{0,H}(t) \quad (14.107)$$

where

$$A_{0,H}(t) = \exp(iH_0 t) A_s \exp(-iH_0 t) \quad (14.108)$$

is the Heisenberg operator corresponding to the Schrödinger operator  $A_s$  when the interaction has been removed. In other words,  $A_{0,H}(t)$  is an interaction picture operator which develops in time according to the relation [see eq. (13.48)]

$$i \frac{d}{dt} A_{0,H}(t) = [A_{0,H}, H_0] \quad (14.109)$$

where  $H_0$  is in the Schrödinger (or interaction) picture.

The relationship between the in- and out-operators defined by eqs. (14.105) is easily established. Extracting  $A_H(t)$  from eq. (14.105a) and substituting into eq. (14.105b) we obtain:

$$A_H^{\text{out}}(t) = \Omega_H^{(-)}(t) \Omega_H^{(+)\dagger}(t) A_H^{\text{in}}(t) \Omega_H^{(+)}(t) \Omega_H^{(-)\dagger}(t). \quad (14.110)$$

Then, using eq. (14.104) and introducing the operator  $S'_s = \Omega_s^{(+)} \Omega_s^{(-)\dagger}$  [note that  $[S'_s, H_s] = 0$  via a unitary transformation of eq. (14.81)], we have

$$A_H^{\text{out}}(t) = S'_s{}^\dagger A_H^{\text{in}}(t) S'_s \quad (14.111)$$

so that the in-operators are transformed into their corresponding out-operators by means of the  $S'_s$  operator. The *exact* equation (14.111) for  $S'_s$  holds independently of the fact that the total Hamiltonian  $H$  may or may not be split into  $H_0$  and  $V$ . For this reason the Heisenberg picture has been used extensively in quantum field theory [22].

Before concluding this section on the collision matrix, we mention several general reviews or books where this subject is treated. These are listed in reference [23] at the end of this chapter.

### 14.3. Green's operators

Let us return to the important relations (14.66). These relations allow us to calculate the state vectors  $\Psi_a^{(\pm)}$ ,  $\Psi_b^{(\pm)}$  or  $\Psi_n^{(\pm)}$  once we know the *Green's operators*

$$G^{(\pm)} = \lim_{\epsilon \rightarrow 0^+} \frac{1}{E - H \pm i\epsilon}. \quad (14.112)$$

The object

$$G(z) = \frac{1}{z - H} \quad (14.113)$$

considered as a function of the complex variable  $z$  is called the *resolvent* of the operator  $H$ . It is a bounded operator in Hilbert space [24] for every value of the variable  $z$  except at the eigenvalues of  $H$ . The Green's operators are thus defined as limits of the resolvent when  $z$  approaches the real axis.

We may also define Green's operators associated respectively to the arrangement channel Hamiltonians  $H_i$  and  $H_f$ , namely

$$G_i^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - H_i \pm i\varepsilon} \quad (14.114a)$$

and

$$G_f^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - H_f \pm i\varepsilon}. \quad (14.114b)$$

More generally, to any arrangement channel Hamiltonian  $H_c$  corresponds the Green's operator

$$G_c^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - H_c \pm i\varepsilon}. \quad (14.114c)$$

In particular, we shall denote by

$$G_0^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - H_0 \pm i\varepsilon} \quad (14.114d)$$

the (completely) free Green's operators corresponding to a channel Hamiltonian  $H_0$  which describes the system when all the particles are free. When we wish to study *direct* collisions (involving no rearrangement) for which  $V_i = V_f = V_d$  we shall find it convenient to use the Green's operators

$$G_d^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - H_d \pm i\varepsilon} \quad (14.114e)$$

with  $H_d = H_i = H_f = H - V_d$ . If  $V_d = V$  (the full interaction between the "elementary" particles which participate to the collision), then the Green's operator (14.114e) simply reduces to the completely free Green's operator (14.114d). In what follows the limit  $\varepsilon \rightarrow 0^+$  will always be implied (unless otherwise stated) so that we shall simplify the notation by writing these various Green's operators as

$$\frac{1}{E - H \pm i\varepsilon}, \quad \frac{1}{E - H_i \pm i\varepsilon}, \quad \text{etc.}$$

Since the Hamiltonians  $H$  and  $H_c$  are Hermitian operators we directly obtain the relations

$$G^{(\pm)\dagger} = G^{(\mp)}; \quad G_c^{(\pm)\dagger} = G_c^{(\mp)}. \quad (14.115)$$

Let us first show that the action of the operators  $G_c^{(\pm)}$  is well defined in that part of Hilbert space corresponding to the continuum spectrum of  $H_c$ . We start from

$$(E - H_c \pm i\varepsilon)\Phi_{c,\gamma} = (E - E_{c,\gamma} \pm i\varepsilon)\Phi_{c,\gamma}. \quad (14.116)$$

Multiplying eq. (14.116) to the left by  $(E - H_c \pm i\varepsilon)^{-1}$ , we obtain

$$\Phi_{c,\gamma} = (E - H_c \pm i\varepsilon)^{-1}(E - E_{c,\gamma} \pm i\varepsilon)\Phi_{c,\gamma}. \quad (14.117)$$

Since  $(E - E_{c,\gamma} \pm i\varepsilon)$  is a number, it can be brought to the left of  $(E - H_c \pm i\varepsilon)^{-1}$ , with the result

$$\frac{1}{E - H_c \pm i\varepsilon} \Phi_{c,\gamma} = \frac{1}{E - E_{c,\gamma} \pm i\varepsilon} \Phi_{c,\gamma}. \quad (14.118)$$

This equation specifies the action of  $G_c^{(\pm)}$  upon an eigenvector belonging to the continuum spectrum of  $H_c$ . It also shows that the eigenvectors  $\Phi_{c,\gamma}$  of  $H_c$  are eigenvectors of  $G_c^{(\pm)}$  with eigenvalues  $(E - E_{c,\gamma} \pm i\varepsilon)^{-1}$ . It is easy to show that the converse is also true. Consider now an arbitrary vector  $|\zeta\rangle$  which may be expanded in the complete set of eigenvectors  $\Phi_\gamma^c$  corresponding to  $H_c$  as

$$|\zeta\rangle = \sum_\gamma a_\gamma \Phi_\gamma^c \quad (14.119)$$

with

$$a_\gamma = \langle \Phi_\gamma^c | \zeta \rangle. \quad (14.120)$$

Here the summation on  $\gamma$  also includes integrals over continuously varying indices, if necessary. Thus

$$\frac{1}{E - H_c \pm i\varepsilon} |\zeta\rangle = \sum_\gamma \frac{1}{E - E_{c,\gamma} \pm i\varepsilon} |\Phi_\gamma^c\rangle \langle \Phi_\gamma^c | \zeta \rangle \quad (14.121)$$

and therefore, since  $|\zeta\rangle$  is an arbitrary vector, we obtain the *spectral representation* of  $G_c^{(\pm)}$ , namely

$$\frac{1}{E - H_c \pm i\varepsilon} = \sum_\gamma \frac{1}{E - E_{c,\gamma} \pm i\varepsilon} |\Phi_\gamma^c\rangle \langle \Phi_\gamma^c|. \quad (14.122)$$

Let us now choose a given *representation*  $\{\lambda\}$  of quantum theory [25]. We then have

$$\left\langle \lambda \left| \frac{1}{E - H_c \pm i\varepsilon} \right| \lambda' \right\rangle = \sum_\gamma \frac{1}{E - E_{c,\gamma} \pm i\varepsilon} \langle \lambda | \Phi_\gamma^c \rangle \langle \Phi_\gamma^c | \lambda' \rangle. \quad (14.123)$$

Now  $\langle \lambda | \Phi_\gamma^c \rangle$  describes the eigenstate  $\Phi_\gamma^c$  in the representation  $\{\lambda\}$ . That is,

$$\Phi_\gamma^c(\lambda) \equiv \langle \lambda | \Phi_\gamma^c \rangle \quad (14.124)$$

is the “wave function” in the  $\{\lambda\}$  representation. Similarly

$$\Phi_\gamma^{c\dagger}(\lambda') \equiv \langle \Phi_\gamma^c | \lambda' \rangle. \quad (14.125)$$

As an example, let us consider the case of non-relativistic potential scattering in the coordinate representation  $\{\mathbf{r}\}$ . We then have

$$\begin{aligned} H_c &\rightarrow H_0 = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2, \\ E &= \hbar^2 k^2/2m, \\ \Phi_{\gamma}^c &\rightarrow \Phi_{\mathbf{k}'}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}' \cdot \mathbf{r}), \\ E_{c,\gamma} &\rightarrow E_{\mathbf{k}'} = \hbar^2 k'^2/2m \end{aligned} \quad (14.126)$$

and

$$\left\langle \mathbf{r} \left| \frac{1}{E - H_0 \pm i\varepsilon} \right| \mathbf{r}' \right\rangle = \int d\mathbf{k}' \frac{1}{E - E_{\mathbf{k}'} \pm i\varepsilon} \langle \mathbf{r} | \Phi_{\mathbf{k}'} \rangle \langle \Phi_{\mathbf{k}'} | \mathbf{r}' \rangle. \quad (14.127)$$

Using eqs. (14.126) and evaluating the integral by the method of Section 5.2, we find that

$$\begin{aligned} \left\langle \mathbf{r} \left| \frac{1}{E - H_0 \pm i\varepsilon} \right| \mathbf{r}' \right\rangle &= \frac{2m}{\hbar^2} \left( -\frac{1}{4\pi} \frac{\exp\{\pm ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \right) \\ &= \frac{2m}{\hbar^2} G_0^{(\pm)}(\mathbf{r}, \mathbf{r}') \end{aligned} \quad (14.128)$$

where  $G_0^{(+)}(\mathbf{r}, \mathbf{r}')$  is the Green's *function*, given by eq. (5.27), which corresponds to an outgoing spherical wave. The other Green's function  $G_0^{(-)}(\mathbf{r}, \mathbf{r}')$ , given by eq. (5.61), obviously yields an *incoming* spherical wave.

We have seen on this example that Green's *functions* are obtained when the corresponding Green's *operators* are "realized" in the coordinate representation. To illustrate this point in a more general case, we consider the Green's operator (14.114c) corresponding to the arrangement channel Hamiltonian

$$H_c = K_c + h_c \quad (14.129)$$

where  $K_c$  is the kinetic energy operator of the arrangement channel  $c$  and  $h_c$  the internal Hamiltonian of that channel. We also have

$$h_c \varphi_{c,n}(\xi_c) = w_{c,n} \varphi_{c,n}(\xi_c). \quad (14.130)$$

Here  $\xi_c$  represents symbolically the set of internal coordinates of the particles in channel  $c$  while  $w_{c,n}$  is their internal energy. The index  $n$  summarizes all the internal quantum numbers. For example, if there are two particles X and Y in channel  $c$ , whose internal quantum states are described respectively by the wave functions  $\varphi_{X,i}(s_X)$  and  $\varphi_{Y,j}(s_Y)$  and if  $h_X$  and  $h_Y$  are the Hamiltonians of these particles such that

$$h_X \varphi_{X,i}(s_X) = w_{X,i} \varphi_{X,i}(s_X) \quad (14.131)$$

and

$$h_Y \varphi_{Y,j}(s_Y) = w_{Y,j} \varphi_{Y,j}(s_Y)$$



we have

$$\begin{aligned} h_c &= h_X + h_Y \\ \varphi_{c,n}(\xi_c) &= \varphi_{X,i}(s_X) \varphi_{Y,j}(s_Y) \end{aligned} \quad (14.132)$$

and

$$w_{c,n} = w_{X,i} + w_{Y,j}.$$

Let us further assume in this particular example that the relative motion is non-relativistic and describe it in the C.M. system of the two colliding particles. Let  $\mathbf{r}_X$  and  $\mathbf{r}_Y$  denote respectively the positions of the centers of mass of X and Y and  $\mathbf{r}_c = \mathbf{r}_X - \mathbf{r}_Y$  their relative vector. We shall also denote the relative momentum by  $\mathbf{p}_c = \hbar \mathbf{k}_c$ , where  $\mathbf{k}_c$  is the relative wave vector. The reduced mass is  $M_c = m_X m_Y / (m_X + m_Y)$ . We may then write the operator  $K_c$  in the coordinate representation as [26],

$$K_c = -\frac{\hbar^2}{2M_c} \nabla_{\mathbf{r}_c}^2. \quad (14.133)$$

The complete set of eigenstates  $\Phi_\gamma^c$  corresponding to  $H_c$  is therefore given by

$$\begin{aligned} \Phi_\gamma^c(\mathbf{r}_c, \xi_c) &= (2\pi)^{-3/2} \exp(i\mathbf{k}_c \cdot \mathbf{r}_c) \varphi_{c,n}(\xi_c) \\ &= (2\pi)^{-3/2} \exp(i\mathbf{k}_c \cdot \mathbf{r}_c) \varphi_{X,i}(s_X) \varphi_{Y,j}(s_Y) \end{aligned} \quad (14.134)$$

where the index  $\gamma$  specifies both  $\mathbf{k}_c$  and the internal quantum number  $n$ , and

$$\begin{aligned} E_{c,\gamma} &= \hbar^2 k_c^2 / 2M_c + w_{c,n} \\ &= \hbar^2 k_c^2 / 2M_c + w_{X,i} + w_{Y,j}. \end{aligned} \quad (14.135)$$

Let us denote by  $Z_c \equiv (\mathbf{r}_c, \xi_c)$  the collection of all the “coordinates” (including spin, isospin . . . coordinates) in channel  $c$ . The Green’s functions  $G_c^{(\pm)}(Z_c, Z'_c)$  corresponding to the Green’s operators  $G_c^{(\pm)}$  are given by

$$G_c^{(\pm)}(Z_c, Z'_c) = \left\langle Z_c \left| \frac{1}{E - H_c \pm i\epsilon} \right| Z'_c \right\rangle. \quad (14.136)$$

Using the spectral representation (14.122) of the Green’s operators, we find that

$$\left\langle Z_c \left| \frac{1}{E - H_c \pm i\epsilon} \right| Z'_c \right\rangle = \sum_\gamma \frac{1}{E - E_{c,\gamma} \pm i\epsilon} \langle Z_c | \Phi_\gamma^c \rangle \langle \Phi_\gamma^c | Z'_c \rangle. \quad (14.137)$$

But

$$\langle Z_c | \Phi_\gamma^c \rangle = \Phi_\gamma^c(Z_c) = (2\pi)^{-3/2} \exp(i\mathbf{k}_c \cdot \mathbf{r}_c) \varphi_{c,n}(\xi_c) \quad (14.138a)$$

and

$$\langle \Phi_\gamma^c | Z'_c \rangle = \Phi_\gamma^{c\dagger}(Z'_c) = (2\pi)^{-3/2} \exp(-i\mathbf{k}_c \cdot \mathbf{r}'_c) \varphi_{c,n}^\dagger(\xi'_c) \quad (14.138b)$$

so that

$$G_c^{(\pm)}(Z_c, Z'_c) = - (2\pi)^{-3} \frac{2M_c}{\hbar^2} \sum_n \int d\mathbf{k}_c \frac{\exp\{i\mathbf{k}_c \cdot (\mathbf{r}_c - \mathbf{r}'_c)\}}{k_c^2 - 2M_c(E - w_{c,n})/\hbar^2 \mp i\epsilon} \varphi_{c,n}(\xi_c) \varphi_{c,n}^\dagger(\xi'_c). \quad (14.139)$$

Setting

$$\kappa_{c,n}^2 = \frac{2M_c}{\hbar^2} (E - w_{c,n}) \quad (14.140)$$

and performing the integral over  $\mathbf{k}_c$  as in Section 5.2 we find that

$$G_c^{(\pm)}(Z_c, Z'_c) = \frac{2M_c}{\hbar^2} \left[ -\frac{1}{4\pi} \sum_n \frac{\exp\{\pm i\kappa_{c,n}|\mathbf{r}_c - \mathbf{r}'_c|\}}{|\mathbf{r}_c - \mathbf{r}'_c|} \varphi_{c,n}(\xi_c) \varphi_{c,n}^\dagger(\xi'_c) \right]. \quad (14.141)$$

We verify easily by using the closure property of the eigenfunctions  $\varphi_{c,n}(\xi_c)$  that

$$(E - H_c)G_c^{(\pm)}(Z_c, Z'_c) = \delta(Z_c, Z'_c) \quad (14.142)$$

where

$$\delta(Z_c, Z'_c) = \delta(\mathbf{r}_c - \mathbf{r}'_c) \delta(\xi_c, \xi'_c) \quad (14.143)$$

is a generalized Kronecker delta symbol.

To illustrate the formulae we have obtained, let us consider the simple case of a channel consisting of a positron and an hydrogen atom in an internal state described by the (non-relativistic) quantum numbers  $(n, l, m)$ .

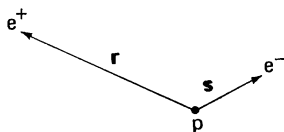


Fig. 14.1. Illustration of the relative coordinate  $\mathbf{r}$  and the internal coordinate  $\mathbf{s}$  used in the text.

We shall assume that the proton is infinitely massive and neglect the spin variables. The relative coordinate is then the vector  $\mathbf{r}_c \equiv \mathbf{r} = \mathbf{r}_{e^+} - \mathbf{r}_p$  and the internal coordinates simply reduce to  $\xi_c \equiv \mathbf{s}$  (see Fig. 14.1). The internal wave functions are the non-relativistic hydrogen atom wave functions  $\psi_{nlm}(\mathbf{s})$  and the corresponding internal energy levels  $w_n$  only depend on the principal quantum number  $n$  within the approximations made here. Thus the Green's function for the channel which we are considering is

$$G_c^{(\pm)}(\mathbf{r}, \mathbf{s}; \mathbf{r}', \mathbf{s}') = \frac{2m_e}{\hbar^2} \left[ -\frac{1}{4\pi} \sum_{nlm} \frac{\exp\{\pm i\kappa_n|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \psi_{nlm}(\mathbf{s}) \psi_{nlm}^*(\mathbf{s}') \right] \quad (14.144)$$

where  $m_e$  is the electron (positron) mass and

$$\kappa_n^2 = \frac{2m_e}{\hbar^2} [E - w_n]. \quad (14.145)$$

It is important to know how to relate the operators  $G^{(\pm)}$  and  $G_c^{(\pm)}$ . This can be done by using the identities between operators

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{A}(B - A)\frac{1}{B} \quad (14.146)$$

and

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{B}(B - A)\frac{1}{A}. \quad (14.147)$$

Choosing

$$\begin{aligned} A &= E - H \pm i\epsilon, \\ B &= E - H_c \pm i\epsilon \end{aligned} \quad (14.148)$$

and using the fact that  $H = H_c + V_c$ , we find from eq. (14.146) that

$$G^{(\pm)} = G_c^{(\pm)} + G^{(\pm)}V_cG_c^{(\pm)} \quad (14.149a)$$

and from eq. (14.147) that

$$G^{(\pm)} = G_c^{(\pm)} + G_c^{(\pm)}V_cG^{(\pm)}. \quad (14.149b)$$

In particular, we have the identities

$$G^{(\pm)} = G_i^{(\pm)} + G^{(\pm)}V_iG_i^{(\pm)} \quad (14.150a)$$

$$G^{(\pm)} = G_i^{(\pm)} + G_i^{(\pm)}V_iG^{(\pm)}, \quad (14.150b)$$

and

$$G^{(\pm)} = G_f^{(\pm)} + G^{(\pm)}V_fG_f^{(\pm)}, \quad (14.151a)$$

$$G^{(\pm)} = G_f^{(\pm)} + G_f^{(\pm)}V_fG^{(\pm)}. \quad (14.151b)$$

Similarly, we have

$$G^{(\pm)} = G_0^{(\pm)} + G^{(\pm)}VG_0^{(\pm)}, \quad (14.152a)$$

$$G^{(\pm)} = G_0^{(\pm)} + G_0^{(\pm)}VG^{(\pm)} \quad (14.152b)$$

and

$$G^{(\pm)} = G_d^{(\pm)} + G^{(\pm)}V_dG_d^{(\pm)}, \quad (14.153a)$$

$$G^{(\pm)} = G_d^{(\pm)} + G_d^{(\pm)}V_dG^{(\pm)} \quad (14.153b)$$

where the Green's operators  $G_0^{(\pm)}$  and  $G_d^{(\pm)}$  are defined respectively by eqs. (14.114d) and (14.114e),  $V$  is the full interaction such that  $H = H_0 + V$  and  $V_d$  is the interaction occurring in a direct collision (no rearrangement). Upon choosing  $A = E - H_c \pm i\epsilon$  and  $B = E - H_0 \pm i\epsilon$  and substituting in eqs. (14.146) and (14.147) we also get

$$G_c^{(\pm)} = G_0^{(\pm)} + G_c^{(\pm)}V^cG_0^{(\pm)} \quad (14.154a)$$

and

$$G_c^{(\pm)} = G_0^{(\pm)} + G_0^{(\pm)}V^cG_c^{(\pm)} \quad (14.154b)$$

with  $V^c = V - V_c$ .

### 14.4. The $T$ -matrix

We define the *transition operator*  $\mathcal{T}_{fi}(E)$  by the relation

$$\mathcal{T}_{fi}(E) = V_i + V_f \frac{1}{E - H + i\varepsilon} V_i. \quad (14.155)$$

Let us first consider the matrix elements of this operator between the asymptotic states  $\Phi_a \equiv \Phi_{i,\alpha}$  and  $\Phi_b \equiv \Phi_{f,\beta}$ , having energies  $E_a = E_b = E$ . These *on-the-energy-shell* transition matrix (or  $T$ -matrix) elements are thus defined as

$$\langle b|\mathcal{T}|a\rangle \equiv \langle f, \beta|\mathcal{T}|i, \alpha\rangle = \langle \Phi_b(E)|\mathcal{T}_{fi}(E)|\Phi_a(E)\rangle. \quad (14.156)$$

Going back to the explicit expressions (14.96) and (14.97) for the  $S$ -matrix elements, we shall now prove that *on the energy shell* ( $E = E_a = E_b$ ) one has

$$\langle b|\mathcal{T}|a\rangle = \langle \Phi_b|V_f|\Psi_a^{(+)}\rangle = \langle \Psi_b^{(-)}|V_i|\Phi_a\rangle \quad (14.157)$$

so that eqs. (14.96) and (14.97) may be written as

$$\langle b|S|a\rangle = \delta_{ba} - 2\pi i\delta(E_a - E_b)\langle b|\mathcal{T}|a\rangle. \quad (14.158)$$

We have already shown above [see eq. (14.98)] that  $\langle \Phi_b|V_f|\Psi_a^{(+)}\rangle = \langle \Psi_b^{(-)}|V_i|\Phi_a\rangle$  on the energy shell. To demonstrate the first equality in eq. (14.157), we observe that, on the energy shell

$$\begin{aligned} \langle \Phi_b|V_i|\Phi_a\rangle &= \langle \Phi_b|H - H_i|\Phi_a\rangle \\ &= \langle \Phi_b|H - E|\Phi_a\rangle \\ &= \langle (H - E)\Phi_b|\Phi_a\rangle \\ &= \langle V_f\Phi_b|\Phi_a\rangle \end{aligned}$$

where we have used the hermiticity of the operators  $H$  and  $V_f$ . Hence

$$\langle \Phi_b|V_i|\Phi_a\rangle = \langle \Phi_b|V_f|\Phi_a\rangle \quad (14.159)$$

and we may use eq. (14.66b) to write, on the energy shell ( $E = E_a = E_b$ )

$$\begin{aligned} \langle \Phi_b|V_f|\Psi_a^{(+)}\rangle &= \left\langle \Phi_b \left| V_f + V_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle \\ &= \left\langle \Phi_b \left| V_i + V_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle \\ &= \langle \Phi_b|\mathcal{T}_{fi}|\Phi_a\rangle = \langle b|\mathcal{T}|a\rangle \end{aligned} \quad (14.160)$$

which completes the proof. We see from eq. (14.158) that the  $T$ -matrix elements  $\langle b|\mathcal{T}|a\rangle$  constitute the “non-trivial” part of the  $S$ -matrix. The matrix elements (14.157) are the multi-channel generalizations of the transition matrix elements (5.43) which we obtained in potential scattering theory. As we have already seen in a simple case [cf. eq. (5.45)], the  $T$ -matrix elements are involved in the computations of the cross sections. This will be shown explicitly in Chapter 15.

Although the on-the-energy-shell  $T$ -matrix elements (14.156) are ultimately the only quantities of physical interest (as we shall see in Chapter 15), it is nevertheless useful to define *off-the-energy-shell* extensions of the  $T$ -matrix elements. Among the infinite number of such extensions, we shall adopt the following definitions

$$\langle b|\mathcal{T}^{(+)}|a\rangle = \langle \Phi_b(E_b)|V_f|\Psi_a^{(+)}(E_a)\rangle, \quad E_a \neq E_b \quad (14.161a)$$

and

$$\langle b|\mathcal{T}^{(-)}|a\rangle = \langle \Psi_b^{(-)}(E_b)|V_i|\Phi_a(E_a)\rangle, \quad E_a \neq E_b. \quad (14.161b)$$

Thus we may write

$$\langle b|\mathcal{T}^{(+)}|a\rangle = \langle \Phi_b(E_b)|\bar{\mathcal{T}}_{fi}(E_a)|\Phi_a(E_a)\rangle \quad (14.162a)$$

and

$$\langle b|\mathcal{T}^{(-)}|a\rangle = \langle \Phi_b(E_b)|\mathcal{T}_{fi}(E_b)|\Phi_a(E_a)\rangle \quad (14.162b)$$

where we have introduced the operator

$$\bar{\mathcal{T}}_{fi}(E) = V_f + V_f \frac{1}{E - H + i\varepsilon} V_i. \quad (14.163)$$

In dealing with several particle dynamics (and in particular with the three-body problem, which we shall study in Chapter 19), it is customary to use a different notation and introduce the *Lovelace operators*

$$U_{fi}(E) \equiv \mathcal{T}_{fi}(E) = V_i + V_i \frac{1}{E - H + i\varepsilon} V_f \quad (14.164a)$$

and

$$\bar{U}_{fi}(E) \equiv \bar{\mathcal{T}}_{fi}(E) = V_f + V_f \frac{1}{E - H + i\varepsilon} V_i. \quad (14.164b)$$

In terms of the Lovelace operators we may obviously rewrite eqs. (14.162) as

$$\langle b|\mathcal{T}^{(+)}|a\rangle = \langle \Phi_b(E_b)|\bar{U}_{fi}(E_a)|\Phi_a(E_a)\rangle \quad (14.165a)$$

and

$$\langle b|\mathcal{T}^{(-)}|a\rangle = \langle \Phi_b(E_b)|U_{fi}(E_b)|\Phi_a(E_a)\rangle. \quad (14.165b)$$

On the energy shell  $E = E_a = E_b$ , these equations reduce to

$$\langle b|\mathcal{T}|a\rangle = \langle \Phi_b(E)|\bar{U}_{fi}(E)|\Phi_a(E)\rangle \quad (14.166a)$$

$$= \langle \Phi_b(E)|U_{fi}(E)|\Phi_a(E)\rangle. \quad (14.166b)$$

We may also define *completely off-the-energy-shell*  $T$ -matrix elements as

$$\begin{aligned} \langle \Phi_b(E_b)|\mathcal{T}_{fi}(E)|\Phi_a(E_a)\rangle &= \langle \Phi_b(E_b)|U_{fi}(E)|\Phi_a(E_a)\rangle \\ &= \left\langle \Phi_b(E_b) \left| V_i + V_i \frac{1}{E - H + i\varepsilon} V_f \right| \Phi_a(E_a) \right\rangle, \\ &E \neq E_a \neq E_b \end{aligned} \quad (14.167a)$$

and

$$\begin{aligned}\langle \Phi_b(E_b) | \bar{\mathcal{T}}_{fi}(E) | \Phi_a(E_a) \rangle &= \langle \Phi_b(E_b) | \bar{U}_{fi}(E) | \Phi_a(E_a) \rangle \\ &= \left\langle \Phi_b(E_b) \left| V_f + V_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a(E_a) \right\rangle, \\ &E \neq E_a \neq E_b. \quad (14.167b)\end{aligned}$$

Evidently,

$$\langle b | \mathcal{T}^{(+)} | a \rangle \rightarrow \langle b | \mathcal{T} | a \rangle \quad \text{as } E_b \rightarrow E_a \quad (14.168a)$$

$$\langle b | \mathcal{T}^{(-)} | a \rangle \rightarrow \langle b | \mathcal{T} | a \rangle \quad \text{as } E_b \rightarrow E_a \quad (14.168b)$$

while

$$\langle \Phi_b(E_b) | \bar{\mathcal{T}}_{fi}(E) | \Phi_a(E_a) \rangle \rightarrow \langle b | \mathcal{T}^{(+)} | a \rangle \quad \text{as } E \rightarrow E_a \quad (14.168c)$$

and

$$\langle \Phi_b(E_b) | \mathcal{T}_{fi}(E) | \Phi_a(E_a) \rangle \rightarrow \langle b | \mathcal{T}^{(-)} | a \rangle \quad \text{as } E \rightarrow E_b. \quad (14.168d)$$

For the particular case of a direct collision ( $V_i = V_f = V_d$ ) we have only to consider the transition operator

$$\mathcal{T}(E) = V_d + V_d \frac{1}{E - H + i\varepsilon} V_d, \quad (14.169)$$

so that the direct transition matrix element is given on the energy shell by

$$\langle b | \mathcal{T} | a \rangle = \left\langle \Phi_b \left| V_d + V_d \frac{1}{E - H + i\varepsilon} V_d \right| \Phi_a \right\rangle. \quad (14.170)$$

Off-the-energy shell extensions of the transition matrix element  $\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | \mathcal{T} | \Phi_a \rangle$  are defined by

$$\begin{aligned}\langle b | \mathcal{T}^{(+)} | a \rangle &= \langle \Phi_b(E_b) | V_d | \Psi_a^{(+)}(E_a) \rangle \\ &= \langle \Phi_b(E_b) | \mathcal{T}(E_a) | \Phi_a(E_a) \rangle\end{aligned} \quad (14.171a)$$

and

$$\begin{aligned}\langle b | \mathcal{T}^{(-)} | a \rangle &= \langle \Psi_b^{(-)}(E_b) | V_d | \Phi_a(E_a) \rangle \\ &= \langle \Phi_b(E_b) | \mathcal{T}(E_b) | \Phi_a(E_a) \rangle\end{aligned} \quad (14.171b)$$

with  $E_a \neq E_b$ . The completely off-the-energy shell  $T$ -matrix element is given by

$$\begin{aligned}\langle \Phi_b(E_b) | \mathcal{T}(E) | \Phi_a(E_a) \rangle &= \left\langle \Phi_b(E_b) \left| V_d + V_d \frac{1}{E - H + i\varepsilon} V_d \right| \Phi_a(E_a) \right\rangle, \\ &E \neq E_a \neq E_b. \quad (14.171c)\end{aligned}$$

Finally, we note that the full  $T$ -operator (which describes transitions such that all the “elementary” particles participating in the collision are free in the initial and final states) is given by

$$\mathcal{T} = V + V \frac{1}{E - H + i\varepsilon} V \quad (14.172)$$

where  $V$  is the full interaction between all the particles.

Let us now return to eq. (14.158). In obtaining this equation we have already taken into account the conservation of energy which appears through the delta function  $\delta(E_a - E_b)$ . We may further reduce the  $S$ -matrix elements by taking into account the conservation of (linear) momentum. If we denote by  $P$  the momentum operator and by  $\mathbf{P}_a$  and  $\mathbf{P}_b$  its eigenvalues in the initial and final asymptotic states such that

$$P\Phi_a = \mathbf{P}_a\Phi_a \quad (14.173a)$$

and

$$P\Phi_b = \mathbf{P}_b\Phi_b \quad (14.173b)$$

we may write the  $S$ -matrix elements (14.158) as

$$\langle b|S|a\rangle = \delta_{ba} - 2\pi i\delta(E_a - E_b)\delta(\mathbf{P}_a - \mathbf{P}_b)T_{ba} \quad (14.174)$$

where the *reduced*  $T$ -matrix element  $T_{ba}$  is now defined on the *energy-momentum shell*. Obviously, if we are describing the collision in the center of mass system, the delta function  $\delta(\mathbf{P}_a - \mathbf{P}_b)$  is unnecessary and we are dealing directly with a reduced  $T$ -matrix  $T_{ba}$  such that the variables of translation are omitted in  $\Phi_a$  and  $\Phi_b$ . This justifies the notation [27] adopted for the  $T$ -matrix elements [see eq. (5.43)] in Part II. Extensions of  $T_{ba}$  off the energy shell may then be defined as for  $\langle b|\mathcal{T}|a\rangle$ . Thus, we have

$$\langle b|\mathcal{T}^{(\pm)}|a\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b)T_{ba}^{(\pm)}(E_b, E_a) \quad (14.175a)$$

$$\langle \Phi_b(E_b)|\mathcal{T}_{fi}(E)|\Phi_a(E_a)\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b)T_{ba}(E_b, E_a, E) \quad (14.175b)$$

and

$$\langle \Phi_b(E_b)|\bar{\mathcal{T}}_{fi}(E)|\Phi_a(E_a)\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b)\bar{T}_{ba}(E_b, E_a, E). \quad (14.175c)$$

For the case of direct scattering there is no distinction between  $\mathcal{T}_{fi}(E)$  and  $\bar{\mathcal{T}}_{fi}(E)$ ; we shall then write

$$\langle \Phi_b(E_b)|\mathcal{T}(E)|\Phi_a(E_a)\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b)T_{ba}(E_b, E_a, E). \quad (14.175d)$$

We note that

$$T_{ba}^{(+)}(E_b, E_a) \rightarrow T_{ba}(E_a) \quad \text{as } E_b \rightarrow E_a, \quad (14.176a)$$

$$T_{ba}^{(-)}(E_b, E_a) \rightarrow T_{ba}(E_a) \quad \text{as } E_b \rightarrow E_a, \quad (14.176b)$$

$$\bar{T}_{ba}(E_b, E_a, E) \rightarrow T_{ba}^{(+)}(E_b, E_a) \quad \text{as } E \rightarrow E_a, \quad (14.176c)$$

$$T_{ba}(E_b, E_a, E) \rightarrow T_{ba}^{(-)}(E_b, E_a) \quad \text{as } E \rightarrow E_b, \quad (14.176d)$$

and, for direct collisions,

$$T_{ba}(E_b, E_a, E) \rightarrow T_{ba}^{(+)}(E_b, E_a) \quad \text{as } E \rightarrow E_a, \quad (14.176e)$$

$$T_{ba}(E_b, E_a, E) \rightarrow T_{ba}^{(-)}(E_b, E_a) \quad \text{as } E \rightarrow E_b. \quad (14.176f)$$

The cases of energy and momentum conservation which lead to eq. (14.174) are two particular examples of the use of constants of the motion to simplify the  $S$  and  $T$  matrices. We shall return to this question in Section 16.7 after having learned how to calculate transition probabilities and cross sections.

## References and notes

- [1] In what follows we shall denote the initial and final arrangement channels of a collision respectively by the indices  $i$  and  $f$ , while  $c$  denotes a general arrangement channel index.
- [2] See GOLDBERGER, M. L. and K. M. WATSON (1964), *Collision Theory* (Wiley, New York) Chapters 3 and 4, where a complete treatment in terms of wave packets is carried out.
- [3] GELL-MANN, M. and M. L. GOLDBERGER (1953), *Phys. Rev.* **91**, 398.
- [4] It is also worth noting that if we imagine the system to be enclosed in a large cubic box of volume  $V = L^3$ , the limiting process  $\epsilon \rightarrow 0^+$  is directly related to the limit  $V \rightarrow \infty$ . Indeed, the colliding particles, having a relative velocity  $v_i$ , cross the box in a time  $\tau_i = L/v_i$ . We must therefore require that the effective duration of time  $\tau_{\text{eff}} = \epsilon^{-1}$  of the wave train be such that  $\tau_{\text{eff}} \ll \tau_i$ . Hence we have  $\epsilon \rightarrow 0^+$  and  $L \rightarrow \infty$  but with  $\epsilon^{-1} \ll L/v_i$ .
- [5] SUNAKAWA, S. (1955), *Progr. Theor. Phys.* **14**, 175.
- [6] LIPPMANN, B. A. and J. SCHWINGER (1950), *Phys. Rev.* **79**, 469.
- [7] MØLLER, C. (1945), *Kgl. Danske Videnskab. Selskab., Mat.-fys. Medd.* **23** (1), [reprinted in *Quantum Scattering Theory*, ed. M. H. Ross, (Indiana University Press, Bloomington, Indiana, 1963)]; (1946), *Kgl. Danske Videnskab. Selskab., Mat.-fys. Medd.* **22** (19).
- [8] FUBINI, S. (1952), *Nuovo Cimento* **9**, 846.
- [9] ECKSTEIN, H. (1954), *Phys. Rev.* **94**, 1063.
- [10] HACK, M. N. (1954), *Phys. Rev.* **96**, 196; (1958), *Nuovo Cimento* **9**, 731.
- [11] We assume here that the interaction does not cause *level shifts* in the continuum. For a discussion of the level shift problem, see for example ref. [2], Chapter 5, Section 5.7.
- [12] In what follows, and in order to simplify the notation we shall omit to write explicitly the kets in equations of the type (14.25).
- [13] In eq. (14.29) it is understood that the symbol  $\delta_{\beta\alpha}$  also implies delta functions of the type  $\delta(\lambda - \lambda')$  for the continuous indices  $\lambda$  and  $\lambda'$  contained respectively in  $\alpha$  and  $\beta$ .
- [14] In writing the rather strange-looking eq. (14.36) we should keep in mind that the operator  $G(z) = (z - H)^{-1}$  is singular for all values of the variable  $z$  corresponding to the eigenvalues of  $H$ . We shall return to this question in Section 14.3.
- [15] GOLDBERGER, M. L. and K. M. WATSON, loc. cit. [2] Sections 4.1, 5.2 and Appendix C.
- [16] NEWTON, R. G. (1966), *Scattering Theory of Waves and Particles* (McGraw-Hill, New York) Chapter 16.
- [17] The concept of the collision matrix ( $S$ -matrix) was introduced independently by WHEELER, J. A. (1937), *Phys. Rev.* **52**, 1107 and HEISENBERG, W. (1943), *Z. Phys.* **120**, 513, 673; (1944), *Z. Phys.* **123**, 93; (1946), *Z. Naturforsch.* **1**, 608. Further important developments were made by MØLLER [7], LIPPMANN and SCHWINGER [6] and GELL-MANN and GOLDBERGER [3]. Early applications of the  $S$ -matrix concept in field theory were made by STUECKELBERG, E. C. G. (1943), *Helv. Phys. Acta* **17**, 3; (1945), **18**, 195; (1946), **19**, 242; SCHWINGER, J. (1948), *Phys. Rev.* **74**, 1439; DYSON, F. J. (1949), *Phys. Rev.* **75**, 486, 1736 and FEYNMAN, R. P. (1949), *Phys. Rev.* **76**, 749, 769; see also FUBINI, S. (1952), *Atti. Accad. Naz. Lincei* **12**, 298. Other important references are MA, S. T. (1953), *Phys. Rev.* **91**, 392; COESTER, F., M. HAMERMESH and K. TANAKA (1954), *Phys. Rev.* **96**, 1142; SUNAKAWA [5]; VAN HOVE, L. (1955), *Physica* **21**, 901; (1956), **22**, 343; ECKSTEIN, H. (1956), *Phys. Rev.* **101**, 880; *Nuovo Cimento* **4**, 1017.
- [18] See for example NEWTON, R. G., loc. cit. [16] Chapter 7; BELINFANTE, F. J. and C. MØLLER (1953), *Kgl. Danske Videnskab. Selskab., Mat.-fys. Medd.* **28** (6). Other



important papers on time-independent formal scattering theory are FEENBERG, E. (1948), Phys. Rev. **74**, 664; GOLDBERGER, M. L. (1951), Phys. Rev. **82**, 757; **84**, 929; HACK [10]; EPSTEIN, S. T. (1955), Phys. Rev. **98**, 196; DE WITT, B. S. (1955), Phys. Rev. **100**, 905.

- [19] A detailed treatment of multi-channel scattering theory may be found in refs. [2] and [16]. See also the original papers of GELL-MANN and GOLDBERGER [3]; ECKSTEIN, H. (1956), Phys. Rev. **101**, 880; LIPPMANN, B. A. (1956), Phys. Rev. **102**, 264; FOLDY, L. and W. TOBOCMAN (1957), Phys. Rev. **105**, 1099; EPSTEIN, S. T. (1957), Phys. Rev. **106**, 598; JAUCH, J. M. (1958), Helv. Phys. Acta **31**, 661; NEWTON, R. G. (1958), Ann. Phys. (N.Y.) **4**, 29; GERJUOY, E. (1958), Ann. Phys. (N.Y.) **5**, 58; COESTER, F. and H. KÜMMEL (1958), Nucl. Phys. **9**, 225; SUNAKAWA, S. (1960), Progr. Theor. Phys. **24**, 963; MITTLEMAN, M. H. (1961), Phys. Rev. **122**, 499, 1930; DAY, T. B., L. S. RODBERG, G. A. SNOW and J. SUCHER (1961), Phys. Rev. **123**, 1051; JORDAN, T. F. (1962), J. Math. Phys. **3**, 414, 429; (1964), **5**, 1345; MITTLEMAN, M. H. (1964), Ann. Phys. (N.Y.) **28**, 430; JOACHAIN, C. J. (1965), Nucl. Phys. **64**, 548; COZ, M. (1965), Nuovo Cimento **35**, 492; Ann. Phys. (N.Y.) **35**, 53; JAUCH, J. M. and J. P. MARCHAND (1966), Helv. Phys. Acta **39**, 325. More recent references dealing with several particle dynamics may be found in Chapters 19, 20 and 21.

- [20] Indeed, let us integrate eq. (14.95) with respect to  $E_b$  over the continuum energy spectrum extending from  $E_0$  to  $\infty$ . If  $E_a > E_0$ , we find that

$$\int_{E_0}^{\infty} \frac{\epsilon}{(E_b - E_a)^2 + \epsilon^2} dE_b = \frac{1}{2}\pi + \tan^{-1} \frac{E_a - E_0}{\epsilon}$$

so that, for  $\epsilon \rightarrow 0^+$

$$C \int_{E_0}^{\infty} \delta(E_b - E_a) dE_b = \frac{1}{2}\pi + \frac{1}{2}\pi = \pi$$

and  $C = \pi$ . The same result obtains for  $E_a = E_0$  since then

$$C \int_0^{\infty} \delta(E) dE = \frac{1}{2}\pi$$

and the integral is equal to  $\frac{1}{2}$  because  $\delta(E)$  is a symmetric function.

- [21] We recall that the operators in the Heisenberg picture are identified by a subscript H.
- [22] A general treatment of formal collision theory, with special emphasis on problems arising in quantum field theory has been given by BRENG, W. and R. HAAG (1959), Fortschr. der Physik **7**, 183 [translated in *Quantum Scattering Theory*, ed. M. H. Ross (Indiana University Press, Bloomington, Indiana, 1963)]. See also ECKSTEIN, H. (1956), Phys. Rev. **101**, 880.
- [23] DE WITT, B. S. (1955), *The Operator Formalism in Quantum Scattering Theory*, University of California Lawrence Radiation Lab. (Berkeley) Report UCRL 2884; JAUCH, J. M. and F. ROHRICH (1955), *The Theory of Photons and Electrons* (Addison-Wesley, Reading, Mass.) Chapters 7 and 8; BRENG and HAAG, loc. cit. [22]; Low, F. E. (1959), in *Brandeis University Summer Institute in Theoretical Physics* (Lecture Notes), p. 3-79; BOGOLUBOV, N. N. and D. V. SHIRKOV (1959), *Introduction to the Theory of Quantized Fields* (Interscience, New York) Chapter 3; HAAG, R. (1961), in *Lectures in Theoretical Physics*, ed. W. E. Brittin (Interscience, New York) Vol. III, p. 326; WU, T. Y. and T. OHMURA (1962), *Quantum Theory of Scattering* (Prentice-Hall, Englewood Cliffs, N.J.) Chapter 4; SCHWEBER, S. S. (1961), *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York) Chapter 11; GOLDBERGER, M. L. and K. M. WATSON, loc. cit. [2] Chapters 3, 4, 5;

MOTT, N. F. and H. S. W. MASSEY (1965), *The Theory of Atomic Collisions* (3d ed. Oxford) Chapters 14, 15;

ROMAN, P. (1965), *Advanced Quantum Theory* (Addison-Wesley, Reading, Mass.) Chapter 4;

NEWTON, R. G. loc. cit. [16] Chapters 6, 7, 16;

BRANDEN, B. H. (1970), *Atomic Collision Theory* (Benjamin, New York) Chapter 4;

TAYLOR, J. R. (1972), *Scattering Theory* (Wiley, New York) Chapters 16–22.

- [24] That is,  $\|Gf\| \leq M\|f\|$  for all vectors  $f$  belonging to the Hilbert space. Here  $\|f\| = (f, f)^{\frac{1}{2}}$  and  $\|Gf\| = (Gf, Gf)^{\frac{1}{2}}$  are respectively the norms of  $f$  and  $Gf$ ; the quantity  $M$  is a constant.
- [25] We recall that such a representation is defined by a complete set of commuting observables (see Appendix A); their common eigenvectors are the basis vectors of the representation.
- [26] In treating this example we shall write explicitly the quantity  $\hbar$ .
- [27] Since we were describing a *one-channel* situation in Part II, we used there the subscripts  $i$  and  $f$  in a straightforward way, i.e.  $T_{fi} = \langle \Phi_{k_f} | V | \psi_{k_i}^{(+)} \rangle$  [cf. eq. (5.43)]. In the *multi-channel* case considered here we need indices  $a$  and  $b$  in  $T_{ba}$  which have an additional content. That is,  $a \equiv (i, \alpha)$  and  $b \equiv (f, \beta)$ .

# Transition Probabilities and Cross Sections

The main topic of this chapter is the calculation of transition probabilities and cross sections from a knowledge of the  $S$ - or  $T$ -matrix elements. This is accomplished in the first two sections. The question of the Lorentz invariance of cross sections is analyzed in Section 15.3. The next section deals with phase space considerations, while Section 15.5 is devoted to the scattering of incoherent beams and the density matrix formalism. Finally, we investigate in Section 15.6 some remarkable consequences of the unitarity property of the  $S$ -matrix, in particular the generalized optical theorem which relates the total (complete) cross section to the imaginary part of the forward elastic scattering amplitude.

## 15.1. Transition probabilities

Let us calculate the probability  $W$  for finding the system at time  $t$  in some “unperturbed” free state  $\Phi_b$ . Using the Schrödinger picture state vector  $\Psi_s(t)$ , we find that

$$W = |\langle \Phi_b \exp(-iE_b t) | \Psi_s(t) \rangle|^2. \quad (15.1)$$

Let  $\Psi_b(t)$  be the interaction picture state vector in the arrangement channel  $f$ . Then

$$\begin{aligned} \Psi_s(t) &= \exp(-iH_f t) \Psi_b(t) \\ &= \exp(-iH_f t) U_f(t, 0) \Psi_b(0) \\ &= \exp(-iH_f t) U_f(t, 0) U_i(0, t') \Psi_a(t') \end{aligned} \quad (15.2)$$

so that

$$W_{ba}(t, t') = |\langle \Phi_b \exp(-iE_b t) | \exp(-iH_f t) U_f(t, 0) U_i(0, t') | \Psi_a(t') \rangle|^2 \quad (15.3)$$

is the probability of finding the system at time  $t$  in the interaction picture free state  $\Phi_b$  when it was described at time  $t'$  by the state vector  $\Psi_a(t')$ . For  $t' \rightarrow -\infty$ ,  $t \rightarrow +\infty$  and after inserting in eq. (15.3) the channel projection operators  $A_i$  and  $A_f$  we find by using eqs. (14.51), (14.52) and (14.85) that the transition probability corresponding to the transition  $a \rightarrow b$  is given by

$$\lim_{\substack{t' \rightarrow -\infty \\ t \rightarrow +\infty}} W_{ba}(t, t') = |\langle b|S|a \rangle|^2. \quad (15.4)$$

In obtaining this result we have used the fact that  $\Psi_a(t') \rightarrow \Phi_a$  as  $t' \rightarrow -\infty$ . We also recall that the indices  $a$  and  $b$  are such that  $a \equiv (i, \alpha)$  and  $b \equiv (f, \beta)$ .

This equation, however, is not very useful since the quantity  $|\langle b|S|a \rangle|^2$  is infinite due to the presence of the energy conserving delta function in eqs. (14.96) or (14.97). In fact, eq. (15.4) simply tells us that an infinite number of transitions  $a \rightarrow b$  occur during an infinite amount of time. The relevant physical question is to ask for the *transition probability per unit time*  $w_{ba}$ , namely [see eq. (15.3)]

$$\begin{aligned} w_{ba} &= \frac{d}{dt} \lim_{t' \rightarrow -\infty} |\langle \Phi_b | U_f(t, 0) U_i(0, t') | \Psi_a(t') \rangle|^2 \\ &= \frac{d}{dt} |\langle \Phi_b | U_f(t, 0) | \Psi_a^{(+)} \rangle|^2 \end{aligned} \quad (15.5)$$

where we have used the fact that  $\Psi_a(t') \rightarrow \Phi_a$  as  $t' \rightarrow -\infty$ , and we recall that  $U_i(0, -\infty) = \Omega_i^{(+)}$ . We may transform eq. (15.5) as follows. We first write

$$\begin{aligned} w_{ba} &= \frac{d}{dt} [\langle \Phi_b | U_f(t, 0) | \Psi_a^{(+)} \rangle \langle \Phi_b | U_f(t, 0) | \Psi_a^{(+)} \rangle^*] \\ &= \langle \Phi_b | \left| \frac{\partial U_f(t, 0)}{\partial t} \right| \Psi_a^{(+)} \rangle \langle \Phi_b | U_f(t, 0) | \Psi_a^{(+)} \rangle^* + \text{c.c.} \end{aligned} \quad (15.6)$$

where c.c. denotes the complex conjugate. Then, using eqs. (13.55) and (13.47) we find that

$$\frac{\partial U_f(t, 0)}{\partial t} = -i V_f(t) U_f(t, 0) = -i \exp(i H_f t) V_f \exp(-i H t) \quad (15.7)$$

and therefore

$$\begin{aligned} w_{ba} &= -i \langle \Phi_b | \exp(i H_f t) V_f \exp(-i H t) | \Psi_a^{(+)} \rangle \\ &\quad \times \langle \Phi_b | \exp(i H_f t) \exp(-i H t) | \Psi_a^{(+)} \rangle^* + \text{c.c.} \\ &= -i [\exp(i E_b t) \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle \exp(-i E_a t)] \\ &\quad \times [\exp(i E_b t) \langle \Phi_b | \Psi_a^{(+)} \rangle \exp(-i E_a t)]^* + \text{c.c.} \\ &= -i \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle \langle \Phi_b | \Psi_a^{(+)} \rangle^* + \text{c.c.} \end{aligned} \quad (15.8)$$

But

$$\begin{aligned}
 \langle \Phi_b | \Psi_a^{(+)} \rangle &= \langle \Psi_b^{(+)} | \Psi_a^{(+)} \rangle + \langle \Phi_b - \Psi_b^{(+)} | \Psi_a^{(+)} \rangle \\
 &= \delta_{ba} - \langle \Phi_b | V_f \frac{1}{E_b - H - i\varepsilon} | \Psi_a^{(+)} \rangle \\
 &= \delta_{ba} - \frac{1}{E_b - E_a - i\varepsilon} \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle
 \end{aligned} \tag{15.9}$$

so that

$$\begin{aligned}
 w_{ba} &= -i \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle \left[ \delta_{ba} - \frac{1}{E_b - E_a + i\varepsilon} \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle^* \right] + \text{c.c.} \\
 &= 2 \operatorname{Im} [\langle \Phi_b | V_f | \Psi_a^{(+)} \rangle] \delta_{ba} \\
 &\quad - i |\langle \Phi_b | V_f | \Psi_a^{(+)} \rangle|^2 \left( \frac{1}{E_b - E_a - i\varepsilon} - \frac{1}{E_b - E_a + i\varepsilon} \right) \\
 &= 2 \operatorname{Im} [\langle \Phi_b | V_f | \Psi_a^{(+)} \rangle] \delta_{ba} + 2 |\langle \Phi_b | V_f | \Psi_a^{(+)} \rangle|^2 \frac{\varepsilon}{(E_b - E_a)^2 + \varepsilon^2}.
 \end{aligned} \tag{15.10}$$

Recalling that [see eq. (14.95)]

$$\lim_{\varepsilon \rightarrow 0^+} \frac{\varepsilon}{(E_b - E_a)^2 + \varepsilon^2} = \pi \delta(E_b - E_a) \tag{15.11}$$

and using eq. (14.157), valid on the energy shell, we find that

$$w_{ba} = 2 \operatorname{Im} \langle b | \mathcal{T} | a \rangle \delta_{ba} + 2\pi \delta(E_b - E_a) |\langle b | \mathcal{T} | a \rangle|^2. \tag{15.12}$$

Now, let us consider a *group* of final states  $\Phi_b$  having almost the same energy as the initial state  $\Phi_a$ . We assume that  $\Phi_a$  does not belong to these states (i.e. we are dealing with a genuine transition) so that the first term on the right of eq. (15.12) disappears. Then the transition probability per unit time  $w$  to the group of states  $\Phi_b$  is given by

$$w = 2\pi \sum_b \delta(E_b - E_a) |\langle b | \mathcal{T} | a \rangle|^2 \tag{15.13}$$

where the summation on  $b$  includes the set of final states which we want to consider. Let us denote by  $\rho_b(E)$  the *density of final states* [so that  $\rho_b dE$  is the number of states  $\Phi_b$  in the energy range  $(E, E + dE)$ ]. Assuming that both  $\rho_b(E)$  and  $\langle b | \mathcal{T} | a \rangle$  are slowly varying functions of  $E$  in the (small) energy range  $(E_b - \Delta E_b, E_b + \Delta E_b)$ , we find that the transition probability per unit time to the group of states  $\Phi_b$  is given by

$$\begin{aligned}
 w &= 2\pi \sum_{b'} \int_{E_b - \Delta E_b}^{E_b + \Delta E_b} \delta(E' - E_a) |\langle b' | \mathcal{T} | a \rangle|^2 \rho_b(E') dE' \\
 &= 2\pi \sum_{b'} \rho_b(E) |\langle b' | \mathcal{T} | a \rangle|^2
 \end{aligned} \tag{15.14}$$

where  $b'$  contains all the indices implied by  $b$  except the energy  $E_b$ , and the  $T$ -matrix element  $\langle b'|\mathcal{T}|a\rangle$  must be evaluated on the energy shell  $E_a = E_b = E$ . Writing explicitly the quantity  $\hbar$  which we had set above equal to unity, we have

$$w = \frac{2\pi}{\hbar} \sum_{b'} \rho_{b'}(E) |\langle b'|\mathcal{T}|a\rangle|^2. \quad (15.15)$$

This formula is very similar to the “golden rule” of time-dependent perturbation theory which we discussed in Chapter 12 [see eq. (12.98)], namely

$$w^{(1)} = \frac{2\pi}{\hbar} \sum_{b'} \rho_{b'}(E) |\langle b'|V|a\rangle|^2 \quad (15.16)$$

where  $w^{(1)}$  is the transition probability per unit time computed to *first order in perturbation theory* so that the potential – acting only once – appears in the matrix element  $\langle b'|V|a\rangle$  instead of the full transition operator.

We may also take into account in eq. (15.13) the conservation of linear momentum. Since

$$\langle b|\mathcal{T}|a\rangle = \delta(\mathbf{P}_b - \mathbf{P}_a) T_{ba} \quad (15.17)$$

we have (with  $\hbar = 1$ )

$$w = 2\pi \sum_b \delta(E_b - E_a) [\delta(\mathbf{P}_b - \mathbf{P}_a)]^2 |T_{ba}|^2. \quad (15.18)$$

We may interpret the object  $[\delta(\mathbf{P}_b - \mathbf{P}_a)]^2$  as follows. Firstly, we note that

$$[\delta(\mathbf{P}_b - \mathbf{P}_a)]^2 = \delta(\mathbf{0}) \delta(\mathbf{P}_b - \mathbf{P}_a). \quad (15.19)$$

Let us enclose the system in a large box of volume  $V$ . We then have [1]

$$\begin{aligned} \delta(\mathbf{0}) \delta(\mathbf{P}_b - \mathbf{P}_a) &\rightarrow (2\pi)^{-3} \int_V d\mathbf{R} \exp(i\mathbf{0} \cdot \mathbf{R}) \delta(\mathbf{P}_b - \mathbf{P}_a) \\ &= \frac{V}{(2\pi)^3} \delta(\mathbf{P}_b - \mathbf{P}_a). \end{aligned}$$

Upon returning to our delta-function normalization, which corresponds to  $V = (2\pi)^3$  we see that

$$\delta(\mathbf{0}) \delta(\mathbf{P}_b - \mathbf{P}_a) \rightarrow \delta(\mathbf{P}_b - \mathbf{P}_a)$$

so that eq. (15.18) becomes

$$w = 2\pi \sum_b \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) |T_{ba}|^2. \quad (15.20)$$

It is worth noting that with our choice of “normalization” for the free waves [see eqs. (5.6)–(5.8)] the particle density is equal to  $(2\pi)^{-3}$  in configuration space. Thus the value of  $w$  which we have obtained is the number of particles scattered into the set of states  $(\Phi_b)$  per unit time and per unit target particle, when there is one incident particle in a volume  $V = (2\pi)^3$ .

## 15.2. Cross sections and lifetimes

Having calculated the transition probability (15.13) from the  $T$ -matrix element, we are now prepared to obtain the corresponding cross sections. Recalling the definition of Section 1.3, we write

$$\Delta\sigma = w/\Phi_A \quad (15.21)$$

where  $\Phi_A$  is the relative flux of the incident particles A with respect to the target. With the "normalization" adopted for the asymptotic states, this quantity is given in both non-relativistic and relativistic cases by

$$\Phi_A = (2\pi)^{-3}v_i = (2\pi)^{-3}|\mathbf{v}_A - \mathbf{v}_B| \quad (15.22)$$

where  $\mathbf{v}_A$  and  $\mathbf{v}_B$  are respectively the (collinear) velocities of the incident particles A and the target particles B and  $v_i$  is the magnitude of the relative velocity in the initial channel. Thus

$$\Delta\sigma = \sum_b \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) \frac{(2\pi)^4}{v_i} |T_{ba}|^2 \quad (15.23)$$

where the sum on  $b$  runs over a range of states determined by the experimental resolution. In particular, if we are interested in transitions  $a \rightarrow b$  from a specific initial channel  $a \equiv (i, \alpha)$ , (with  $i$  and  $\alpha$  fixed) to some final states  $b \equiv (f, \beta)$  belonging to the arrangement channel  $f$ , we may write

$$\Delta\sigma = \sum_\beta \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) \frac{(2\pi)^4}{v_i} |T_{ba}|^2 \quad (15.24)$$

where the summation includes a set of final states  $\beta$  belonging to the arrangement channel  $f$  and having the internal quantum numbers which are contained in the index  $\beta$  [2].

In order to specify the summation over the range of final states which appears in eq. (15.23) or (15.24), we consider for example a collision of the type



in which there are  $n$  distinct particles in the final state with wave vectors  $\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n$ , internal quantum numbers  $\alpha_1, \alpha_2, \dots, \alpha_n$  and energies  $E_1, E_2, \dots, E_n$ . Because of our normalization (5.6)–(5.8) of free states, the number of states in the interval  $(\mathbf{k}, \mathbf{k} + d\mathbf{k})$  is  $d\mathbf{k}$ . Thus the *phase space element* in the final state is  $d\mathbf{k}_1 \cdot d\mathbf{k}_2 \dots d\mathbf{k}_n$  and we may rewrite eq. (15.23) as

$$\Delta\sigma = \sum_{\alpha_1, \alpha_2, \dots, \alpha_n} \int d\mathbf{k}_1 d\mathbf{k}_2 \dots d\mathbf{k}_n \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) \frac{(2\pi)^4}{v_i} |T_{ba}|^2. \quad (15.26)$$

We note that the dynamics of the process is entirely contained in the transition matrix element  $T_{ba}$  while the phase space factors are of a purely kinematical nature. The range of variables over which the sums or integrations in eq. (15.26) are performed depends on the resolution of the detectors. For example, if the experimental setting cannot distinguish the spins of the

outgoing particles – so that all are counted indistinctly by the detectors – one must sum over final spins. Similarly, eq. (15.26) must be integrated over the momenta and summed over the other quantum numbers of the final particles corresponding to the collision (15.25) but which cannot be detected by the experimental apparatus.

If the range of the sum over final states is very small, we may replace  $\Delta\sigma$  by the differential  $d\sigma$ . When, on the contrary, the summation includes all the possible final states, then  $\Delta\sigma = \sigma_{\text{tot}}$ , the *total* cross section for all processes that can be generated from the interaction of the two initial particles. By summing over all possible final states within a given final channel [3]  $b \equiv (f, \beta)$ , we obtain from eq. (15.26) the total cross section  $\sigma_{ba}^{\text{tot}}$  for the transition from channel  $a \equiv (i, \alpha)$  to channel  $b \equiv (f, \beta)$ .

The cross sections given by eq. (15.26) are those corresponding to the case where the two colliding particles A and B are in specific internal states before the collision. Frequently, however, these two particles are distributed among a *mixture* of states, so that the observed cross sections are obtained by performing a weighted average of eq. (15.26) over the initial quantum numbers of the particles A and B. For example, if the colliding particles have spins  $S_A$  and  $S_B$  and are *randomly* distributed over the set of  $(2S_A + 1)(2S_B + 1)$  spin states – in which case the scattering system is said to be *unpolarized* – the average differential cross section is

$$d\bar{\sigma} = \frac{1}{(2S_A + 1)(2S_B + 1)} \sum_{S_A, S_B} d\sigma^{(S_A, S_B)} \quad (15.27)$$

where  $d\sigma^{(S_A, S_B)}$  is the differential cross section for the case when particles A and B are respectively in the spin states denoted by  $S_A$  and  $S_B$ . When the spin states are not randomly distributed, the scattering system is said to be *polarized*. We shall examine examples of such polarized systems in Sections 15.5 and 18.3.

The cross section formulae which we have obtained are not correct when there are *identical* particles in the initial or final states. In this case, a proper symmetrization of the initial and final asymptotic states must be performed. A simple example is provided by a collision in which  $N$  identical elementary particles emerge in the final state. Then, in order to avoid counting the same states repeatedly, we must write for the total cross section

$$\sigma_{\text{tot}} = \frac{1}{N!} \int d\sigma. \quad (15.28)$$

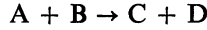
Similarly, if there are  $N_i (i = 1, 2, \dots, n)$  identical elementary particles of the kind  $i$  in the final state, then

$$\sigma_{\text{tot}} = \frac{1}{\prod_{i=1}^n (N_i!)} \int d\sigma. \quad (15.29)$$



The scattering of identical particles will be considered in more detail in Section 16.6.

Let us now return to eq. (15.26) and illustrate this formula on a simple example, namely the collision



where we assume that the particles A, B, C and D are “elementary” and distinct. We shall describe this collision in the center of mass system, and denote the rest mass, wave vector, energy and spin of the particles A, B, C, D respectively by  $m_A, \mathbf{k}_A, E_A, S_A$ ;  $m_B, \mathbf{k}_B, E_B, S_B$ ; etc. The differential cross section corresponding to the case where the internal states are well defined is (writing explicitly the quantity  $\hbar$ )

$$d\sigma = \frac{(2\pi)^4}{\hbar v_i} \int d\mathbf{k}_C d\mathbf{k}_D \delta(E_b - E_a) \delta(\mathbf{k}_C + \mathbf{k}_D) |T_{ba}|^2 \quad (15.30)$$

where  $v_i$  is the relative incident velocity. After integration over  $\mathbf{k}_D$  we find that eq. (15.30) may be rewritten as

$$d\sigma = \frac{(2\pi)^4}{\hbar v_i} \int d\mathbf{k}_f \delta(E_b - E_a) |T_{ba}|^2 \quad (15.31)$$

where the reduced  $T$ -matrix element is given explicitly by

$$T_{ba} = \langle S_C, S_D | T(\mathbf{k}_f, \mathbf{k}_i) | S_A, S_B \rangle. \quad (15.32)$$

Here

$$\mathbf{k}_i = \mathbf{k}_A = -\mathbf{k}_B \quad (15.33)$$

is the initial relative wave vector in the C.M. system [see eqs. (2.17) or (2.97)] while

$$\mathbf{k}_f = \mathbf{k}_C = -\mathbf{k}_D \quad (15.34)$$

is the final relative wave vector in the C.M. system. The second equality in eq. (15.33) follows from the fact that  $\mathbf{k}_A + \mathbf{k}_B = 0$  in the C.M. system, while the second equality in eq. (15.34) is due to the momentum conserving delta function in eq. (15.30).

In order to take into account the energy-conserving delta function in eq. (15.30) we write

$$d\mathbf{k}_f = k_f^2 dk_f d\Omega = \rho_b(E_b) dE_b d\Omega \quad (15.35)$$

where  $d\Omega$  is an element of solid angle into which the vector  $\mathbf{k}_f$  is pointing and

$$\rho_b(E_b) = k_f^2 dk_f / dE_b \quad (15.36)$$

is the density of final states per unit energy. For a relativistic collision such that

$$\begin{aligned} E_b &= E_C + E_D \\ &= c(m_C^2 c^2 + \hbar^2 |\mathbf{k}_C|^2)^{1/2} + c(m_D^2 c^2 + \hbar^2 |\mathbf{k}_D|^2)^{1/2} \\ &= c(m_C^2 c^2 + \hbar^2 |\mathbf{k}_f|^2)^{1/2} + c(m_D^2 c^2 + \hbar^2 |\mathbf{k}_f|^2)^{1/2} \end{aligned} \quad (15.37)$$

we have (with  $k_f \equiv |k_f|$ )

$$dE_b/dk_f = \hbar^2 c^2 k_f [1/E_C + 1/E_D] \quad (15.38)$$

so that

$$\rho_b(E_b) = \frac{k_f}{\hbar^2 c^2 (1/E_C + 1/E_D)}. \quad (15.39)$$

Returning to eq. (15.31), we now integrate over the variable  $E_b$ , keeping  $d\Omega$  fixed. We obtain in this way the differential cross section for emission of the particle C in the direction  $\Omega$ , namely

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \rho_b(E) |T_{ba}|^2 \quad (15.40)$$

or

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \frac{k_f}{\hbar^2 c^2 (1/E_C + 1/E_D)} |T_{ba}|^2 \quad (15.41)$$

where the right-hand side must be evaluated on the energy shell

$$E = E_b = E_a = E_A + E_B = E_C + E_D. \quad (15.42)$$

The non-relativistic limit of eq. (15.41) is easily obtained since in this case

$$\frac{1}{E_C} + \frac{1}{E_D} = \frac{1}{m_C c^2} + \frac{1}{m_D c^2} = \frac{1}{M_f c^2} \quad (15.43)$$

where  $M_f = m_C m_D / (m_C + m_D)$  is the reduced mass in the final channel. Then

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \frac{k_f M_f}{\hbar^2} |T_{ba}|^2. \quad (15.44)$$

We verify that since the non-relativistic energy of the relative motion is given in the final channel by

$$E_b = \hbar^2 k_f^2 / 2M_f \quad (15.45)$$

we have indeed

$$\rho_b(E_b) = k_f^2 dk_f / dE_b = k_f M_f / \hbar^2. \quad (15.46)$$

We may still transform eq. (15.44) as follows. Remembering that for a non-relativistic motion

$$v_i = \hbar k_i / M_i \quad (15.47)$$

where  $M_i = m_A m_B / (m_A + m_B)$  is the reduced mass in the initial channel, we have

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{M_i M_f}{\hbar^4} \frac{k_f}{k_i} |T_{ba}|^2. \quad (15.48)$$

In analogy with the simple case of potential scattering, it is convenient to introduce a *scattering amplitude*  $f_{ba}$  which, except for a phase, is defined by the formula

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} |f_{ba}|^2 \quad (15.49)$$

where  $d\sigma/d\Omega$  is the C.M. differential cross section given by eq. (15.40). Thus

$$|f_{ba}|^2 = \frac{(2\pi)^4 k_i}{\hbar v_i} \rho_b(E) |T_{ba}|^2. \quad (15.50)$$

In the relativistic case we may use eq. (15.39) and the fact that

$$v_i = \frac{dE_a}{\hbar dk_i} = \hbar c^2 k_i \left[ \frac{1}{E_A} + \frac{1}{E_B} \right] \quad (15.51)$$

to find that

$$f_{ba} = \frac{(2\pi)^2}{\hbar^2 c^2} \frac{(E_A E_B E_C E_D)^{1/2}}{E} T_{ba} e^{i\phi} \quad (15.52)$$

where  $E = E_A + E_B$  is the total energy in the C.M. system and  $\phi$  is an arbitrary phase.

When the scattering is non-relativistic we deduce directly from the comparison of eqs. (15.48) and (15.49) that

$$f_{ba} = \frac{(2\pi)^2}{\hbar^2} (M_i M_f)^{1/2} T_{ba} e^{i\phi}. \quad (15.53)$$

If we choose  $\phi = \pi$  we find that

$$f_{ba} = - \frac{(2\pi)^2}{\hbar^2} (M_i M_f)^{1/2} T_{ba} \quad (15.54)$$

so that in the particular case of potential scattering, where  $M_i = M_f = m$ , the formula (15.54) exactly reduces to the result (5.44) which we obtained in Section 5.3. In what follows we shall adopt the choice  $\phi = \pi$ .

So far, we have discussed collisions of the type (15.25), with two particles A and B in the initial state. Our discussion may be extended to the case where there are  $m$  particles in the initial channel. We shall not treat explicitly the situation where  $m \geq 3$  but examine instead the special case  $m = 1$ . This is a *decay* process of the type

$$X \rightarrow C_1 + C_2 + \cdots + C_n. \quad (15.55)$$

The transition probability per unit time for such a process is still given by eq. (15.20). The *lifetime*  $\tau$  of the initial state is thus defined by

$$\tau = 1/W \quad (15.56)$$

where

$$W = \frac{2\pi}{2S_X + 1} \sum_{S_X} \sum_{\alpha_1, \alpha_2, \dots, \alpha_n} \int dk_1 dk_2 \dots dk_n \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) |T_{ba}|^2 \quad (15.57)$$

is the *total* transition probability per unit time, averaged over the internal quantum numbers (e.g. the spin  $S_X$ ) of the decaying (unpolarized) system X, and summed over the final internal quantum numbers and momenta of the outgoing particles. We shall return to eq. (15.57) in the next section. We note here that when there are many different modes of decay, the lifetime  $\tau$  is such that

$$\frac{1}{\tau} = W = \sum_i W_i = \sum_i \frac{1}{\tau_i} \quad (15.58)$$

where  $\tau_i$  is the partial lifetime for decay into channel  $i$ .

### 15.3. Lorentz invariance

Before we examine the behaviour of cross sections and transition matrix elements under Lorentz transformations, let us return once more to the definition of cross sections given in Section 1.3. We consider a beam of particles A directed towards a target consisting of  $n_B$  particles B. Let us assume that the detector registers the particles C and that the counting rate, i.e. the number of particles C detected per unit time is  $\Delta N_C$  for a given range of final states. This counting rate is proportional to the incoming flux  $\Phi_A$  and to the number of scatterers  $n_B$ . Thus

$$\Delta N_C = \Delta\sigma(AB \rightarrow C \dots)n_B\Phi_A \quad (15.59)$$

where the proportionality constant is the cross section for the production of particles C in collisions of particles A with particles B within the given range of final states. If the target is at rest before the collision, we have

$$\Phi_A = \rho_A(v_A)_L \quad (15.60)$$

where  $\rho_A$  is the density of beam particles and  $(v_A)_L$  the magnitude of their velocity in the laboratory system. We note that with the normalization convention for free waves which we adopted above the beam particle density is just  $\rho_A = (2\pi)^{-3}$ . It will prove convenient in what follows to adopt another normalization for free waves so that we shall use directly eq. (15.60) to calculate the incident flux.

Let us transform eq. (15.59) in such a way that the symmetry between the two colliding particles is more apparent. For that purpose, we write

$$n_B = \rho_B V \quad (15.61)$$

where  $\rho_B$  is the particle density of the target and  $V$  the effective target volume interacting with the incident beam. Then, with the help of eqs. (15.60) and (15.61), eq. (15.59) becomes

$$\Delta\sigma = \frac{\Delta N_C/V}{\rho_A \rho_B (v_A)_L} \quad (15.62)$$

and we note that  $(v_A)_L$  is the relative velocity of particles A and B. We shall also define the object

$$F = \rho_A \rho_B (v_A)_L \quad (15.63)$$

together with the quantity

$$\Delta \tilde{N}_C = \Delta N_C / V \quad (15.64)$$

which is the number of particles C detected per unit time and per unit volume (i.e. per unit four dimensional volume). Thus

$$\Delta \sigma = \Delta \tilde{N}_C / F. \quad (15.65)$$

We note that because of the Lorentz-Fitzgerald contraction of lengths [4] we have (with  $c = 1$ )

$$\rho_A = \rho_A^0 [1 - (v_A)_L^2]^{-1/2} \quad (15.66)$$

where  $\rho_A^0$  is the beam particle density in its rest frame. Thus

$$F = \rho_A^0 \rho_B^0 (v_A)_L [1 - (v_A)_L^2]^{-1/2}. \quad (15.67)$$

We now examine the scattering process in another Lorentz frame which moves with respect to the laboratory system with a uniform velocity. Since  $\Delta \tilde{N}_C$  is a number of particles per unit four-dimensional volume, it is *invariant* under Lorentz transformations. We assume that the motion of the new frame is parallel to  $(v_A)_L$ , with the velocity  $u$ , in such a way that the target has the velocity  $-u$  in the new frame, while the beam particles have velocities whose magnitude is given by

$$v'_A = \frac{(v_A)_L - u}{1 - (v_A)_L u}. \quad (15.68)$$

Since

$$F' = \rho'_A \rho'_B (v'_A + u) \quad (15.69)$$

we have

$$\begin{aligned} F' &= \rho_A^0 \rho_B^0 (v'_A + u) (1 - v'^2_A)^{-1/2} (1 - u^2)^{-1/2} \\ &= \rho_A^0 \rho_B^0 (v_A)_L [1 - (v_A)_L^2]^{-1/2} = F \end{aligned} \quad (15.70)$$

so that  $F$  is invariant under proper Lorentz transformations parallel to the axis along which the collinear velocities of the beam and target particles are directed. Hence the cross section (15.65) which is the ratio of the two invariant quantities  $\Delta \tilde{N}_C$  and  $F$  is also invariant under these Lorentz transformations.

We now want to consider collision processes in Lorentz frames such that the velocities of the two colliding particles are not collinear. In this case the definition of cross sections is not obvious. Given the Lorentz invariance property for collinear velocities, it is convenient to *define* the cross sections

to be invariant under *all* proper Lorentz transformations [5]. To this end we need an invariant generalization of  $F$  which we obtain in the following way. Since (with  $\hbar = c = 1$ )

$$(v_A)_L = |\mathbf{k}_A|_L / (E_A)_L \quad (15.71)$$

and

$$\rho_A = \rho_A^0 [1 - (v_A)_L^2]^{-1/2} = \rho_A^0 (E_A)_L / m_A \quad (15.72)$$

we deduce from eq. (15.63) that in the laboratory system

$$F = \rho_A^0 \frac{(E_A)_L}{m_A} \rho_B^0 \frac{|\mathbf{k}_A|_L}{(E_A)_L} = \rho_A^0 \rho_B^0 \frac{|\mathbf{k}_A|_L}{m_A}. \quad (15.73)$$

We now introduce the "triangle function" (2.100) and use the fact that the magnitude of the wave vector of particle A in the laboratory system is given by

$$|\mathbf{k}_A|_L = \frac{1}{2m_B} \sqrt{\lambda(s, m_A^2, m_B^2)} \quad (15.74)$$

to write the quantity  $F$  in invariant form as

$$F = \rho_A^0 \rho_B^0 \sqrt{\lambda(s, m_A^2, m_B^2)} / 2m_A m_B. \quad (15.75)$$

With  $F$  given by eq. (15.75), the cross section (15.65) is invariant for all proper Lorentz transformations.

Let us now return to the formula (15.26) and try to recast it into a form which exhibits explicitly Lorentz invariance properties. We first note that if  $\mathbf{k}$  and  $E$  are respectively the wave vector and energy of a particle in the original Lorentz frame, while  $\mathbf{k}'$  and  $E'$  are their values in a new Lorentz frame moving with a velocity  $\mathbf{u}$  with respect to the first, we have

$$d\mathbf{k}/E = d\mathbf{k}'/E'. \quad (15.76)$$

Indeed, let the velocity  $\mathbf{u}$  be parallel to the  $z$  axis, so that eq. (2.106) – which relates the four-momenta of the particle in the two frames – applies. Then, with  $\mathbf{v}' = \mathbf{k}'/E'$  ( $\hbar = c = 1$ ), we have

$$\begin{aligned} dk_x &= dk'_x, & dk_y &= dk'_y, \\ dk_z &= \gamma[dk'_z + u dE'] = \gamma[dk'_z + u d\mathbf{k}' \cdot \mathbf{v}'] \end{aligned}$$

so that the Jacobian  $J(\partial\mathbf{k}'/\partial\mathbf{k})$  is given by

$$J\left(\frac{\partial\mathbf{k}'}{\partial\mathbf{k}}\right) = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \gamma uv'_x & \gamma uv'_y & \gamma(1 + uv'_z) \end{vmatrix} = \gamma(1 + \mathbf{u} \cdot \mathbf{v}').$$

Hence

$$d\mathbf{k} = \gamma(1 + \mathbf{u} \cdot \mathbf{v}') d\mathbf{k}'. \quad (15.77)$$

Since we also have

$$E = \gamma(E' + u k'_z) = \gamma(E' + uv'_z E') = \gamma(1 + \mathbf{u} \cdot \mathbf{v}') E' \quad (15.78)$$

we see that eqs. (15.77) and (15.78) imply eq. (15.76).

In what follows we shall denote the quantity  $d\mathbf{k}/E$  as the (one-particle) *Lorentz invariant phase space* [6]. We may introduce explicitly these invariant quantities in eq. (15.26) and write

$$\Delta\sigma = \sum_{\alpha_1, \alpha_2, \dots, \alpha_n} \int \frac{d\mathbf{k}_1}{E_1} \frac{d\mathbf{k}_2}{E_2} \dots \frac{d\mathbf{k}_n}{E_n} \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) \times \frac{(2\pi)^4}{E_A E_B v_i} |\sqrt{E_1 E_2 \dots E_n} T_{ba} \sqrt{E_A E_B}|^2 \quad (15.79)$$

where we have also factored out the product  $E_A E_B$ . With the help of eq. (15.74) we note that in the laboratory system

$$E_A E_B v_i = (E_A)_L m_B \frac{|\mathbf{k}_A|_L}{(E_A)_L} = m_B |\mathbf{k}_A|_L = \frac{1}{2} \sqrt{\lambda(s, m_A^2, m_B^2)}. \quad (15.80)$$

Thus, introducing the invariant expression

$$B = \frac{1}{2} \sqrt{\lambda(s, m_A^2, m_B^2)} \quad (15.81)$$

we may recast eq. (15.79) into the form

$$\Delta\sigma = \sum_{\alpha_1, \alpha_2, \dots, \alpha_n} \int \frac{d\mathbf{k}_1}{E_1} \frac{d\mathbf{k}_2}{E_2} \dots \frac{d\mathbf{k}_n}{E_n} \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) \times \frac{(2\pi)^4}{B} |\sqrt{E_1 E_2 \dots E_n} T_{ba} \sqrt{E_A E_B}|^2. \quad (15.82)$$

Since the quantities  $\Delta\sigma$ ,  $d\mathbf{k}_i/E_i$ ,  $B$  and the four-dimensional delta function

$$\delta^4(P_b - P_a) = \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a)$$

are all Lorentz invariants, we conclude that the object

$$M_{ba} = \sqrt{E_1 E_2 \dots E_n} T_{ba} \sqrt{E_A E_B} \quad (15.83)$$

is also a Lorentz invariant [7], which we call the (Møller) invariant transition matrix [8]. In terms of this quantity we may write eq. (15.81) as

$$\Delta\sigma = \sum_{\alpha_1, \alpha_2, \dots, \alpha_n} \int \frac{d\mathbf{k}_1}{E_1} \frac{d\mathbf{k}_2}{E_2} \dots \frac{d\mathbf{k}_n}{E_n} \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) \frac{(2\pi)^4}{B} |M_{ba}|^2. \quad (15.84)$$

To conclude this section we comment briefly on the formula (15.57) which corresponds to the decay process (15.55). Introducing the invariant transition matrix

$$M_{ba} = \sqrt{E_1 E_2 \dots E_n} T_{ba} \sqrt{E_X} \quad (15.85)$$

we write (with  $\hbar = 1$ )

$$\frac{1}{\tau} = W = \quad (15.86)$$

$$\frac{2\pi}{2S_X + 1} \frac{1}{E_X} \sum_{S_X} \sum_{\alpha_1, \alpha_2, \dots, \alpha_n} \int \frac{d\mathbf{k}_1}{E_1} \frac{d\mathbf{k}_2}{E_2} \dots \frac{d\mathbf{k}_n}{E_n} \delta(E_b - E_a) \delta(\mathbf{P}_b - \mathbf{P}_a) |M_{ba}|^2.$$

The integral being Lorentz invariant, the transformation property of the lifetime  $\tau$  is the same as that of  $E_X$ , the energy of the decaying particle.

Hence, if  $\tau_0$  is the lifetime of the particle in its own Lorentz rest frame, we have in a new Lorentz frame moving with a velocity  $u$  with respect to the first,

$$\tau = \tau_0(1 - \beta^2)^{-1/2}, \quad \beta = u/c. \quad (15.87)$$

This is known as the *time dilatation* effect. For the case of a two-body decay  $X \rightarrow C_1 + C_2$  in the rest frame of the decaying particle  $X$  (of rest mass  $m_X$ ), we have  $E_X = m_X$  and the integral in eq. (15.86) is easily reduced with the result

$$\frac{1}{\tau} = \frac{2\pi}{2S_X + 1} \frac{k_f}{m_X^2} 4\pi \sum_{S_X} \sum_{S_1, S_2} |M_{ba}|^2 = \frac{8\pi^2}{2S_X + 1} \frac{k_f}{m_X^2} \sum_{S_X} \sum_{S_1, S_2} |M_{ba}|^2 \quad (15.88)$$

where  $k_f$  is the relative final wave vector, while  $S_1$  and  $S_2$  are respectively the spins of the particles  $C_1$  and  $C_2$ .

### 15.4. Phase space considerations

We have already seen above that the volume of the (non-invariant) phase space corresponding to wave vectors between  $k$  and  $k + dk$  is  $dk$  (with our normalization (5.6)–(5.8) for free states). Thus the non-invariant  $n$ -particle phase space (Nips) volume element is simply

$$dNips(k_1, k_2, \dots, k_n) = \prod_{i=1}^n dk_i. \quad (15.89)$$

For relativistic collisions, it is convenient to introduce a Lorentz invariant phase space (Lips). For one particle we have shown above that it is given by (or proportional to)  $dk/E$ , so that the  $n$ -particle Lorentz invariant phase space volume element may be chosen to be

$$dLips(k_1, k_2, \dots, k_n) = \prod_{i=1}^n dk_i/E_i \quad (15.90)$$

where  $k_1, k_2, \dots$  now denote the corresponding four-vectors [9].

It is important to note from eq. (15.26) or (15.84) that the integration over final momenta is always restricted by energy and momentum conservation. We can incorporate this feature into the definitions of the phase space volume elements. For example, we may define the restricted non-invariant phase space element (with  $\hbar = 1$ ) as

$$dNips(E, P, k_1, k_2, \dots, k_n, E_1, E_2, \dots, E_n) = \delta(E - \sum_i E_i) \delta^3(P - \sum_i k_i) \prod_{i=1}^n dk_i \quad (15.91)$$

where  $P$  is the total momentum and  $E$  the total energy. Similarly, the restricted Lorentz invariant phase space element is given by

$$dLips(s; k_1, k_2, \dots, k_n) = \delta^4(P - \sum_i k_i) dLips(k_1, k_2, \dots, k_n) \quad (15.92)$$



where  $P$  is the total four-momentum and the dependence on  $P$  only occurs through the quantity  $s = P^2$  since  $d\text{Lips}$  is Lorentz-invariant. We note that in the center of mass system eq. (15.91) becomes

$$dN_{\text{ips}}(E, k_1, k_2, \dots k_n, E_1, E_2, \dots E_n) = \delta(E - \sum_i E_i) \delta^3(\sum_i k_i) \prod_{i=1}^n dk_i \quad (15.93)$$

while eq. (15.92) yields

$$d\text{Lips}(s, k_1, k_2, \dots k_n) = \delta(\sqrt{s} - \sum_i E_i) \delta^3(\sum_i k_i) d\text{Lips}(k_1, k_2, \dots k_n). \quad (15.94)$$

Let us now return to the basic relation (15.26) or (15.84). We have already pointed out that if some final particles are unobserved, an integration must be performed over their momenta and a summation over their other possible quantum numbers. If we assume for a moment that  $T_{ba}$  (or  $M_{ba}$ ) is independent of these variables, we see that *phase space integrals* of the type

$$\int dk_1 dk_2 \dots dk_n \delta(E - \sum_i E_i) \delta^3(P - \sum_i k_i) \quad (15.95)$$

or

$$\int \frac{dk_1}{E_1} \frac{dk_2}{E_2} \dots \frac{dk_n}{E_n} \delta^4(P - \sum_i k_i) \quad (15.96)$$

must be evaluated [10]. Since the dynamics is entirely contained in the matrix elements  $T_{ba}$  (or  $M_{ba}$ ), we note that phase space integrals only produce *kinematical effects*; they yield in fact a “background” corresponding to the behaviour of the system if  $T_{ba}$  (or  $M_{ba}$ ) were constant. Hence the genuine *dynamical effects* only appear by a comparison of the integrals evaluated with and without the presence of  $|T_{ba}|^2$  (or  $|M_{ba}|^2$ ).

### 15.5. Scattering systems in mixed states. The density matrix

We have only considered so far the scattering of particles which may be described by a single state vector, i.e. a ray in Hilbert space. Such systems are said to be in a *pure* state. They are prepared in a specific way, their state vector being obtained by performing a *maximal measurement* in which all values of a complete set of commuting observables have been ascertained.

In many cases, however, the measurement made on the system is *not* maximal. For example, a beam of particles may be prepared in such a way that certain quantum numbers are only known through a probability distribution. Such systems, which cannot be represented by a single ray in Hilbert space are said to be in *mixed states*. The description of these systems is conveniently made in terms of the *density matrix formalism* of statistical mechanics [11–13]. This method has also the advantage of treating pure and mixed systems on the same footing.

### 15.5.1. General properties of the density matrix

Let us first present the density matrix in a general way. We consider a system which consists of an ensemble of subsystems  $\alpha = 1, 2, \dots, N$ . We suppose that each of the subsystems is in a pure state and is therefore characterized by a distinct state vector  $\Psi^{(\alpha)}$  which we may expand into orthonormal eigenvectors  $\psi_n$  of some complete set of operators. Using Dirac's notation so that we denote the state vector  $\Psi^{(\alpha)}$  by  $|\alpha\rangle$  and the basis states  $\psi_n$  by  $|n\rangle$ , we have

$$|\alpha\rangle = \sum_n c_n^{(\alpha)} |n\rangle \quad (15.97)$$

with

$$\begin{aligned} \langle n' | n \rangle &= \delta_{n'n} \quad \text{or} \quad \delta(n' - n), \\ c_n^{(\alpha)} &= \langle n | \alpha \rangle \end{aligned} \quad (15.98)$$

and

$$\sum_n |c_n^{(\alpha)}|^2 = 1.$$

Consider now a physical quantity  $\mathcal{A}$  represented by an operator  $A$ . The expectation value of this operator in the pure state  $\Psi^{(\alpha)}$  is given by

$$\langle A \rangle_\alpha = \langle \alpha | A | \alpha \rangle = \sum_n \sum_{n'} c_n^{(\alpha)*} c_{n'}^{(\alpha)} \langle n' | A | n \rangle \quad (15.99)$$

and therefore its average value over the ensemble is

$$\langle A \rangle = \sum_{\alpha=1}^N P_\alpha \langle A \rangle_\alpha \quad (15.100)$$

where  $P_\alpha$  is the *statistical weight factor* for the system  $\alpha$ , i.e. the probability of obtaining this system among the ensemble. The quantities  $P_\alpha$  must therefore be such that

$$0 \leq P_\alpha \leq 1 \quad (15.101)$$

and

$$\sum_{\alpha=1}^N P_\alpha = 1. \quad (15.102)$$

Writing eq. (15.100) explicitly with the help of eq. (15.99), we find that

$$\langle A \rangle = \sum_{\alpha=1}^N P_\alpha \sum_n \sum_{n'} c_n^{(\alpha)*} c_{n'}^{(\alpha)} \langle n' | A | n \rangle \quad (15.103)$$

or

$$\langle A \rangle = \sum_{\alpha=1}^N \sum_n \sum_{n'} \langle n | \alpha \rangle P_\alpha \langle \alpha | n' \rangle \langle n' | A | n \rangle. \quad (15.104)$$

This suggests that we introduce the *density operator*

$$\rho = \sum_{\alpha=1}^N |\alpha\rangle P_\alpha \langle \alpha| \quad (15.105)$$

and the *density matrix*

$$\begin{aligned} \rho_{nn'} &\equiv \langle n | \rho | n' \rangle = \sum_{\alpha=1}^N P_\alpha c_{n'}^{(\alpha)*} c_n^{(\alpha)} \\ &= \sum_{\alpha=1}^N \langle n | \alpha \rangle P_\alpha \langle \alpha | n' \rangle \end{aligned} \quad (15.106)$$

in terms of which we can recast eq. (15.104) into the form

$$\begin{aligned}\langle A \rangle &= \sum_n \sum_{n'} \langle n | \rho | n' \rangle \langle n' | A | n \rangle \\ &= \sum_n \langle n | \rho A | n \rangle = \text{Tr}(\rho A)\end{aligned}\quad (15.107)$$

where  $\text{Tr}$  denotes the trace. Thus *the knowledge of  $\rho$  enables us to compute the statistical average of  $A$* . We note immediately from eq. (15.105) that the eigenvectors of  $\rho$  are just the possible pure states of the ensemble, while its eigenvalues are the corresponding statistical weights  $P_\alpha$ . We also remark that the special case  $A = I$  yields the normalization condition

$$\text{Tr} \rho = 1. \quad (15.108)$$

The diagonal matrix elements of  $\rho$  have a very simple physical interpretation. Indeed, the quantity

$$\langle n | \rho | n \rangle = \sum_{\alpha=1}^N P_\alpha |c_n^{(\alpha)}|^2 \quad (15.109)$$

gives the probability of finding a member of the ensemble in the state  $n$ .

Let us establish a few additional properties of the density operator. We first note from eq. (15.105) that  $\rho$  is *Hermitian*, namely

$$\rho = \rho^\dagger \quad (15.110a)$$

or

$$\langle n | \rho | n' \rangle = \langle n' | \rho | n \rangle^*. \quad (15.110b)$$

Therefore the density matrix may always be diagonalized by a unitary transformation.

Next, we note from eqs. (15.101) and (15.109) that

$$\rho_{nn} = \langle n | \rho | n \rangle \geq 0 \quad (15.111)$$

so that  $\rho$  is a *positive semidefinite* operator. In fact, combining eqs. (15.108) and (15.111), we see that all the diagonal matrix elements of  $\rho$  lie between 0 and 1. That is,

$$0 \leq \rho_{nn} \leq 1. \quad (15.112)$$

Let us choose a representation in which  $\rho$  is diagonal, so that  $\rho_{nn'} = \rho_{nn} \delta_{nn'}$ . Then, using eqs. (15.108) and (15.112), we have

$$\text{Tr}(\rho^2) \leq \text{Tr} \rho = 1 \quad (15.113)$$

and this relation holds true in any representation because the trace is invariant under a basis transformation. We note that since  $\rho$  is Hermitian [see eqs. (15.110)] we may also write eq. (15.113) as

$$\sum_n \sum_{n'} |\rho_{nn'}|^2 \leq 1. \quad (15.114)$$

We now consider a particular case such that the system is in a *pure state*  $|\lambda\rangle$ . Then  $P_\alpha = \delta_{\alpha\lambda}$  and we infer from eq. (15.105) that

$$\rho^\lambda = |\lambda\rangle\langle\lambda|. \quad (15.115)$$

Hence in this case the density operator becomes a *projection operator* such that

$$(\rho^\lambda)^2 = \rho^\lambda \quad (15.116)$$

and therefore we have now

$$\text{Tr}(\rho^\lambda)^2 = \text{Tr} \rho^\lambda = 1. \quad (15.117)$$

Because  $P_\alpha = \delta_{\alpha\lambda}$  for a pure state, we also note that eqs. (15.104) and (15.107) reduce in this case to

$$\langle A \rangle = \text{Tr}(\rho A) = \langle \lambda | A | \lambda \rangle. \quad (15.118)$$

If we elect to work in a representation such that  $\rho^\lambda$  is diagonal, we infer from eq. (15.118) that

$$\rho_{nn'}^\lambda = \delta_{n\lambda} \delta_{n'\lambda} \quad (15.119)$$

and therefore the only non-vanishing element of  $\rho_{nn'}^\lambda$  is the diagonal element in the  $\lambda$ th row and column, which is equal to one. Hence, all the *eigenvalues* of the pure state density operator  $\rho^\lambda$  are zero, except only one which is equal to unity. This last property is obviously independent of the basis choice and may thus be used to characterize the density matrix of a pure state.

Until now, we have labelled the rows and columns of the density matrix  $\rho_{nn'}$  by simple indices  $n$  and  $n'$ . In general, of course, the symbol  $n$  refers to a collection of indices. Some of these may take on discrete values, others may vary continuously. Thus in general we should write

$$\rho_{nn'} \equiv \rho_{n_1, n_2, \dots; n'_1, n'_2, \dots} \quad (15.120)$$

In many cases, however, we are interested in some particular property of the system (spin, isospin, energy, . . .). We then keep only the relevant indices and define in that way a *reduced density matrix*. It is clear that by using reduced density matrices we lose all information about the variables which are disregarded.

### 15.5.2. The density matrix for a spin- $\frac{1}{2}$ system -

As an illustration of the general methods outlined above, let us consider the simple case of an "elementary" particle having a spin  $s = \frac{1}{2}$ . We shall denote by  $(p_x, p_y, p_z)$  the eigenvalues of the three components of the momentum of the particle, while  $|p_x p_y p_z\rangle$  is the corresponding eigenvector. Writing the spin functions as  $\chi_v$ , we also have

$$S^2 \chi_v = s(s+1) \hbar^2 \chi_v \quad (15.121)$$

and

$$S_z \chi_v = v \hbar \chi_v. \quad (15.122)$$

Here  $S$  is the spin operator of the particle and  $S_z = S \cdot \hat{u}$ , where  $\hat{u}$  is a unit vector along an axis which we choose as our  $z$ -axis. The eigenvalue  $v$  refers to the *spin orientation* of the particle; it can only take the two values  $v = \pm \frac{1}{2}$ .

Using the Dirac notation we shall also write the spin states along some direction as  $|v\rangle \equiv |\chi_v\rangle$ .

The possible pure states of the particle may be labelled by the eigenvalues  $p_x, p_y, p_z$  and  $v$ , so that the density matrix elements read in this case

$$\langle n|\rho|n'\rangle = \langle p_x, p_y, p_z, v|\rho|p'_x, p'_y, p'_z, v'\rangle. \quad (15.123)$$

We note that the momentum indices are continuous, while the spin indices are discrete. If we are only interested in the spin properties, we can disregard the momentum labels and focus our attention on the *reduced density matrix*  $\langle v|\rho|v'\rangle$ , which is a  $2 \times 2$  matrix in spin space. Because the unit  $2 \times 2$  matrix

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (15.124)$$

and the three Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (15.125)$$

form a complete set of  $2 \times 2$  matrices, we may write the density matrix as

$$\rho = a_0 I + a_x \sigma_x + a_y \sigma_y + a_z \sigma_z \quad (15.126)$$

where the quantities  $a_0, a_x, a_y, a_z$  are four complex parameters. We may also use a slightly different notation and write eq. (15.126) as

$$\rho = a_0 I + \sum_{i=1}^3 a_i \sigma_i = a_0 I + \mathbf{a} \cdot \boldsymbol{\sigma} \quad (15.127)$$

with  $\mathbf{a} \equiv (a_x, a_y, a_z)$  or  $(a_1, a_2, a_3)$  and  $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$  or  $(\sigma_1, \sigma_2, \sigma_3)$ . Because  $\text{Tr } \rho = 1$ ,  $\text{Tr } I = 2$  and  $\text{Tr } \sigma_i = 0$ , we see that

$$a_0 = \frac{1}{2}. \quad (15.128)$$

To understand the meaning of  $a_i$  ( $i = 1, 2, 3$ ), let us calculate the average value of  $\sigma_i$ . According to eq. (15.107) we have

$$\langle \sigma_i \rangle = \text{Tr}(\rho \sigma_i). \quad (15.129)$$

Using eq. (15.127) together with the fact that  $\text{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$ , we find that

$$\langle \sigma_i \rangle = 2a_i. \quad (15.130)$$

Hence, eq. (15.127) becomes

$$\rho = \frac{1}{2}(I + \boldsymbol{\sigma} \cdot \mathbf{P}) \quad (15.131)$$

where we have introduced the *polarization vector*

$$\mathbf{P} = \langle \boldsymbol{\sigma} \rangle. \quad (15.132)$$

Using the explicit representation (15.125) of the Pauli spin matrices, we may also write eq. (15.131) as

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + P_3 & P_1 - iP_2 \\ P_1 + iP_2 & 1 - P_3 \end{pmatrix}. \quad (15.133)$$

In order to give a simple physical interpretation to the polarization vector  $\mathbf{P}$ , let us diagonalize  $\rho$ . We obtain in this way

$$\rho = \begin{pmatrix} \frac{1}{2}(1 + P) & 0 \\ 0 & \frac{1}{2}(1 - P) \end{pmatrix} \quad (15.134)$$

where the quantity  $P = \pm |\mathbf{P}|$  may be obtained from the equation

$$P^2 = 1 - 4 \det \rho \quad (15.135)$$

in which  $\det \rho$  denotes the determinant of the density matrix. Comparison of eqs. (15.133) and (15.134) shows that in the representation where  $\rho$  is diagonal we have

$$P_1 = P_2 = 0, \quad P = P_3. \quad (15.136)$$

Moreover, in that representation we see from eq. (15.131) that  $\boldsymbol{\sigma} \cdot \mathbf{P}$  is also diagonal. If we denote by  $|\chi_\uparrow\rangle$  and  $|\chi_\downarrow\rangle$  the kets corresponding to spin “up” and spin “down” with  $\mathbf{P}$  as the  $z$ -axis, we may write

$$\boldsymbol{\sigma} \cdot \mathbf{P} |\chi_\uparrow\rangle = P |\chi_\uparrow\rangle \quad (15.137a)$$

and

$$\boldsymbol{\sigma} \cdot \mathbf{P} |\chi_\downarrow\rangle = -P |\chi_\downarrow\rangle. \quad (15.137b)$$

Returning to eq. (15.134), and remembering that the eigenvalues of  $\rho$  are precisely the statistical weights, we see that the quantities  $\frac{1}{2}(1 + P)$  and  $\frac{1}{2}(1 - P)$  are the probabilities of finding in the mixture the pure states with spin “up” and spin “down”, respectively. Hence  $P$  is equal to the probability of finding the system in the state  $|\chi_\uparrow\rangle$ , minus that of finding it in the state  $|\chi_\downarrow\rangle$ . In other words, if we write a general spin function for the system as

$$|\chi_v\rangle = a_+ |\chi_\uparrow\rangle + a_- |\chi_\downarrow\rangle \quad (15.138)$$

we have

$$P = |a_+|^2 - |a_-|^2. \quad (15.139)$$

We note that when  $P = 0$  we have an equal mixture of states with spin “up” and spin “down”. Then  $\rho = \frac{1}{2}I$ , the two statistical weights are equal to  $\frac{1}{2}$  and the system is said to be *completely unpolarized*. On the contrary, when the system is in a *pure state*, we have  $\rho^2 = \rho$  [see eq. (15.116)] which implies from eq. (15.131) that

$$\frac{1}{4}[I + 2\boldsymbol{\sigma} \cdot \mathbf{P} + (\boldsymbol{\sigma} \cdot \mathbf{P})^2] = \frac{1}{4}(I + 2\boldsymbol{\sigma} \cdot \mathbf{P} + P^2 I) = \frac{1}{2}(I + \boldsymbol{\sigma} \cdot \mathbf{P}) \quad (15.140)$$

or  $P^2 = 1$ . Hence there are *two* pure states corresponding to the values  $P = +1$  and  $P = -1$ , respectively. These states are called *completely polarized*. For such pure states  $|\pm \frac{1}{2}\rangle$  having a spin orientation  $\pm \frac{1}{2}$  in the  $z$ -direction we may write the density matrices as

$$\rho_{\text{pol}, +1/2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{for } P = +1 \quad (15.141a)$$

and

$$\rho_{\text{pol}, -1/2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{for } P = -1. \quad (15.141b)$$

Furthermore, if we adopt the vector  $\mathbf{P}$  with  $P = +1$  as our  $z$ -axis, we see that eqs. (15.137) now reduce to

$$\sigma_z |\pm \tfrac{1}{2}\rangle = \pm |\tfrac{1}{2}\rangle \quad (15.142)$$

as they should.

We have examined above the extreme cases of completely unpolarized and completely polarized beams, corresponding respectively to the values  $|\mathbf{P}| = 0$  and  $|\mathbf{P}| = 1$ . For all intermediate values of  $|\mathbf{P}|$  such that  $0 < |\mathbf{P}| < 1$  the system is said to be *partially polarized*. In this case we have

$$\tfrac{1}{2} < \text{Tr}(\rho^2) = \tfrac{1}{2}(1 + P^2) < 1. \quad (15.143)$$

Since  $\text{Tr}(\rho^2) = 1$  corresponds to a completely polarized (pure) state and  $\text{Tr}(\rho^2)$  is an increasing function of  $|\mathbf{P}|$ , it is natural to call  $|\mathbf{P}|$  the *degree of polarization of the system*.

To conclude the examination of this simple example, let us return to the parametrization of the density matrix. From eq. (15.133) we note that for a spin- $\frac{1}{2}$  system in a *mixed state* the (reduced)  $2 \times 2$  density matrix is entirely specified by the *three* real independent parameters  $(P_1, P_2, P_3)$ . Thus in this case we need *three independent measurements* to determine the density matrix and therefore the state of the system. More generally, if the density matrix is an  $m \times m$  matrix, it is a simple matter to deduce from eqs. (15.108) and (15.110) that it is specified by  $m^2 - 1$  parameters. For example, in the case of a particle having spin 1 we have  $m = 3$  so that 8 independent measurements are required to determine its state.

If we now specialize to the case of *pure states*, we remark that additional constraints are imposed on the density matrix. Thus for a spin- $\frac{1}{2}$  system the quantity  $P^2 = P_1^2 + P_2^2 + P_3^2 = 1$  so that only *two* independent parameters remain. For the case of an  $m \times m$  matrix the fact that the system is in a pure state implies  $(m - 1)^2$  constraints so that only  $2m - 2$  independent measurements must be made.

### 15.5.3. Collision processes and the density matrix

Let us now apply the density matrix formalism to the description of a collision experiment. To this end, we shall consider the system made of the “beam” and the “target” to be a *statistical ensemble* [14] of subsystems. Each of these subsystems contains a pair of particles, i.e. a “beam” particle and a “target” particle. We shall assume that the system is initially in a *mixed state* described by the density matrix  $\rho_i$ , and we want to express the scattering cross section in terms of  $\rho_i$ .

In order to orient ourselves, it is convenient to consider first the scattering of “elementary” particles A and B, having respectively the spins  $S_A, S_B$  and the spin orientations  $v_A, v_B$  along a given axis. For example, if the system of “beam” particles A and “target” particles B is prepared in such a way that it

is unpolarized, the (reduced) density operator  $\rho_i$  (referring to spin variables) is given by

$$\rho_i = \frac{1}{(2S_A + 1)(2S_B + 1)} I \quad (15.144)$$

where  $I$  is the unit operator and we are working in a  $(2S_A + 1)(2S_B + 1)$ -dimensional spin space. More generally, if we denote by  $\chi^{(\alpha)}$  the initial spin state of the pair  $\alpha$  in the representation in which  $\rho_i$  is diagonal, we may write from eq. (15.105)

$$\rho_i = \sum_{\alpha=1}^N |\chi^{(\alpha)}\rangle P_{i,\alpha} \langle \chi^{(\alpha)}| \quad (15.145)$$

where  $P_{i,\alpha}$  is the fraction of the subsystems being initially in the state  $\chi^{(\alpha)}$ .

Let us suppose that the same particles A and B emerge in the final state, with spin orientations  $v'_A$  and  $v'_B$  respectively. The reduced transition matrix element for a scattering process  $(\mathbf{k}_i, v_A, v_B) \rightarrow (\mathbf{k}_f, v'_A, v'_B)$  (where  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are respectively the initial and final relative wave vectors) may then be written explicitly as

$$T_{ba} = \langle \mathbf{k}_f, v'_A, v'_B | T | \mathbf{k}_i, v_A, v_B \rangle \quad (15.146)$$

with  $k = |\mathbf{k}_i| = |\mathbf{k}_f|$ . Since we are interested in the transitions between the spin states it is convenient to introduce a generalized scattering amplitude defined by the relation

$$\langle v'_A, v'_B | M | v_A, v_B \rangle = -(2\pi)^2 k \frac{dk}{dE} \langle \mathbf{k}_f, v'_A, v'_B | T | \mathbf{k}_i, v_A, v_B \rangle. \quad (15.147)$$

Then, using eqs. (15.40), (15.36) and (15.51), we see that the differential cross section for a transition  $(v_A, v_B) \rightarrow (v'_A, v'_B)$  is given by

$$\frac{d\sigma}{d\Omega} (v_A, v_B \rightarrow v'_A, v'_B) = |\langle v'_A, v'_B | M | v_A, v_B \rangle|^2. \quad (15.148)$$

If we are considering scattering processes leading from an initial unpolarized system to specific final spin orientations  $(v'_A, v'_B)$ , we have from eq. (15.27)

$$\frac{d\sigma}{d\Omega} (v'_A, v'_B) = \frac{1}{(2S_A + 1)(2S_B + 1)} \sum_{v_A, v_B} |\langle v'_A, v'_B | M | v_A, v_B \rangle|^2 \quad (15.149)$$

or

$$\frac{d\sigma}{d\Omega} (v'_A, v'_B) = \langle v'_A, v'_B | M \rho_i M^\dagger | v'_A, v'_B \rangle \quad (15.150)$$

where we have used eq. (15.144) and the fact that

$$\langle v_A, v_B | M^\dagger | v'_A, v'_B \rangle = \langle v'_A, v'_B | M | v_A, v_B \rangle^*. \quad (15.151)$$



Finally, the differential cross section for an unpolarized initial system and for any final spin orientation (i.e. such that we do not measure any spin orientations) is simply

$$\frac{d\bar{\sigma}}{d\Omega} = \sum_{v'_A, v'_B} \frac{d\sigma}{d\Omega}(v'_A, v'_B) \quad (15.152)$$

or

$$\frac{d\bar{\sigma}}{d\Omega} = \sum_{v'_A, v'_B} \langle v'_A, v'_B | M \rho_i M^\dagger | v'_A, v'_B \rangle. \quad (15.153)$$

But this is just

$$\frac{d\bar{\sigma}}{d\Omega} = \text{Tr}(M \rho_i M^\dagger) \quad (15.154)$$

where the trace is evaluated in the  $(2S_A + 1)(2S_B + 1)$ -dimensional spin space.

The interesting feature of eq. (15.154) is that *it is valid for any polarization of the initial system*. Indeed, let us choose the representation  $\chi$  in which the initial density matrix is diagonal. The cross section for a pair  $\alpha$  of particles in the ensemble is then given by

$$\frac{d\sigma^{(\alpha)}}{d\Omega} = \sum_{\chi'} |\langle \chi' | M | \chi^{(\alpha)} \rangle|^2 \quad (15.155)$$

where we recall that  $\chi^{(\alpha)}$  denotes the initial spin state of the pair  $\alpha$  in the representation which diagonalizes  $\rho_i$ . The average cross section for the entire system made of  $N$  pairs of beam and target particles is then given by

$$\begin{aligned} \frac{d\bar{\sigma}}{d\Omega} &= \sum_{\alpha=1}^N P_{i,\alpha} \frac{d\sigma^{(\alpha)}}{d\Omega} \\ &= \sum_{\alpha} \sum_{\chi'} P_{i,\alpha} \langle \chi' | M | \chi^{(\alpha)} \rangle \langle \chi^{(\alpha)} | M^\dagger | \chi' \rangle \\ &= \text{Tr}(M \rho_i M^\dagger) \end{aligned}$$

where we have used eq. (15.145). This is precisely the result given by eq. (15.154).

We may also obtain the density matrix  $\rho_f$  describing the system in the final state. Keeping the initial spin states  $\chi^{(\alpha)}$  in which  $\rho_i$  is diagonal, we note that the final (unnormalized) spin states arising from  $\chi^{(\alpha)}$  are given by  $M|\chi^{(\alpha)}\rangle$ . Hence, the final density operator  $\rho_f$  may be obtained from eq. (15.145) by replacing each  $\chi^{(\alpha)}$  by  $M\chi^{(\alpha)}$ . This yields

$$\rho_f = \frac{M \rho_i M^\dagger}{\text{Tr}(M \rho_i M^\dagger)} \quad (15.156)$$

where the denominator ensures that the normalization condition  $\text{Tr } \rho_f = 1$  is observed. In fact, we may also use eq. (15.154) to write

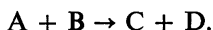
$$\rho_f = \frac{M \rho_i M^\dagger}{d\bar{\sigma}/d\Omega} \quad (15.157)$$

It is worth noting that the above results do not depend on the particular representation  $\chi$  used to describe the incident beam. We also remark that the expression (15.157) describes the final system corresponding to scattering in a *given* direction  $\mathbf{k}_f$ . More explicitly we should write

$$\rho_{\mathbf{k}_f}(S_A, S_B) = \frac{M(\mathbf{k}_i, \mathbf{k}_f, S_A, S_B) \rho_{\mathbf{k}_i}(S_A, S_B) M^\dagger(\mathbf{k}_i, \mathbf{k}_f, S_A, S_B)}{\text{Tr}[M^\dagger(\mathbf{k}_i, \mathbf{k}_f, S_A, S_B) \rho_{\mathbf{k}_i}(S_A, S_B) M(\mathbf{k}_i, \mathbf{k}_f, S_A, S_B)]} \quad (15.158)$$

and interpret  $\text{Tr}(M \rho_i M^\dagger)$  as a *partial trace* in which the final directions of the particles are fixed.

It is a simple matter to generalize the above results for two-body *reactions* of the type



Let us denote the initial and final center of mass energies respectively by  $E_i(k_i)$  and  $E_f(k_f)$ . Calling  $S_C$  and  $S_D$  the spins of the particles C and D in the final channel, and  $v_C$  and  $v_D$  their spin orientation, we may define the generalized scattering amplitude

$$\langle v_C, v_D | M | v_A, v_B \rangle = -(2\pi)^2 \left[ k_i k_f \frac{dk_i}{dE_i} \frac{dk_f}{dE_f} \right]^{1/2} \langle f; \mathbf{k}_f, v_C, v_D | T | i; \mathbf{k}_i, v_A, v_B \rangle. \quad (15.159)$$

More explicitly, the object  $M$  may be written as  $M(i, f; \mathbf{k}_i, \mathbf{k}_f; S_A, S_B; S_C, S_D)$  and it is now in general a rectangular  $(2S_A + 1)(2S_B + 1) \times (2S_C + 1)(2S_D + 1)$  matrix in spin space. A straightforward generalization of the foregoing discussion then yields the average differential cross section

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{k_f}{k_i} \text{Tr}(M \rho_i M^\dagger) \quad (15.160)$$

while  $\rho_f$  is still given by eq. (15.156). The initial density matrix is evidently a (square) matrix of order  $(2S_A + 1)(2S_B + 1)$ , but the final (square) density matrix  $\rho_f$  is now of order  $(2S_C + 1)(2S_D + 1)$ .

We have shown thus far how to use the density matrix to study binary collisions involving "elementary" particles with spin. However, it is clear from the discussion of Section 15.5.1 that the density matrix formalism may be used to analyze more general collisions and (or) various aspects of scattering processes related to other variables (energy, isospin, etc.). The simple formulae which we have obtained above for two-particle scattering will be illustrated in Chapter 18 for the special case of spin  $\frac{1}{2}$ -spin 0 scattering.

## 15.6. Unitarity relations and the optical theorem

We have already established in Section 14.2 the fundamental property of unitarity of the  $S$ -matrix. We shall now investigate the consequences of this unitarity property for the transition matrix elements.

Let us start from eq. (14.158), namely

$$\langle b|S|a\rangle = \delta_{ba} - 2\pi i\delta(E_b - E_a)\langle b|\mathcal{T}|a\rangle \quad (15.161)$$

and express the unitarity property (14.87). That is,

$$\sum_n \langle b|S^\dagger|n\rangle\langle n|S|a\rangle = \delta_{ba} \quad (15.162)$$

and

$$\sum_n \langle b|S|n\rangle\langle n|S^\dagger|a\rangle = \delta_{ba}. \quad (15.163)$$

Let us focus our attention on this last equation. Using eq. (15.161) together with the fact that  $\langle n|S^\dagger|a\rangle = \langle a|S|n\rangle^*$ , we find that

$$\sum_n [\delta_{nb} - 2\pi i\delta(E_n - E_b)\langle b|\mathcal{T}|n\rangle] [\delta_{na} + 2\pi i\delta(E_n - E_a)\langle a|\mathcal{T}|n\rangle^*] = \delta_{ba} \quad (15.164)$$

or

$$\begin{aligned} \delta_{ba} - 2\pi i\delta(E_a - E_b)\langle b|\mathcal{T}|a\rangle + 2\pi i\delta(E_b - E_a)\langle a|\mathcal{T}|b\rangle^* \\ + 4\pi^2 \sum_n \delta(E_n - E_b)\delta(E_n - E_a)\langle b|\mathcal{T}|n\rangle\langle a|\mathcal{T}|n\rangle^* = \delta_{ba} \end{aligned} \quad (15.165)$$

so that

$$\begin{aligned} i\delta(E_b - E_a)[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] \\ = 2\pi\delta(E_a - E_b) \sum_n \delta(E_n - E_a)\langle b|\mathcal{T}|n\rangle\langle a|\mathcal{T}|n\rangle^*. \end{aligned} \quad (15.166)$$

This equation is trivially satisfied when  $E_b \neq E_a$ . However, on the energy shell  $E = E_a = E_b$ , we have

$$i[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] = 2\pi \sum_n \delta(E - E_n)\langle b|\mathcal{T}|n\rangle\langle a|\mathcal{T}|n\rangle^*. \quad (15.167a)$$

Similarly, by developing eq. (15.162) in the same way, one obtains

$$i[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] = 2\pi \sum_n \delta(E - E_n)\langle n|\mathcal{T}|b\rangle^*\langle n|\mathcal{T}|a\rangle. \quad (15.167b)$$

These very important non-linear equations are called *the unitarity relations of the  $T$  matrix*. Completely similar equations obviously hold for the reduced  $T$ -matrix elements on the energy-momentum shell. Thus

$$i[T_{ba} - T_{ab}^*] = 2\pi \sum_n \delta(E - E_n)\delta(\mathbf{P}_n - \mathbf{P}_a)T_{bn}T_{an}^* \quad (15.168a)$$

and

$$i[T_{ba} - T_{ab}^*] = 2\pi \sum_n \delta(E - E_n)\delta(\mathbf{P}_n - \mathbf{P}_a)T_{nb}^*T_{na} \quad (15.168b)$$

are the *unitarity relations for the reduced  $T$  matrix elements*.

We may also write the unitarity relations in *operator form*. Indeed, from eq. (15.167b) we infer that

$$i(\mathcal{T}_{fi} - \mathcal{T}_{fi}^\dagger) = 2\pi\mathcal{T}_{fi}^\dagger\delta(E - H_c)\mathcal{T}_{fi} \quad (15.169a)$$

while eq. (15.167a) yields

$$i(\mathcal{T}_{fi} - \mathcal{T}_{fi}^\dagger) = 2\pi\mathcal{T}_{fi}\delta(E - H_c)\mathcal{T}_{fi}^\dagger \quad (15.169b)$$

where the transition operator  $\mathcal{T}_{fi}$  is defined by eq. (14.155) and where  $H_c$  is a channel Hamiltonian with “free” eigenvectors  $|\Phi_{c,r}\rangle \equiv |\Phi_n\rangle \equiv |n\rangle$ . If there is only one arrangement channel, so that the total Hamiltonian of the system may be split as  $H = H_0 + V$ , then eqs. (15.169) reduce to

$$i(\mathcal{T} - \mathcal{T}^\dagger) = 2\pi\mathcal{T}^\dagger\delta(E - H_0)\mathcal{T} \quad (15.170a)$$

or

$$i(\mathcal{T} - \mathcal{T}^\dagger) = 2\pi\mathcal{T}\delta(E - H_0)\mathcal{T}^\dagger \quad (15.170b)$$

with  $\mathcal{T} = V + V(E - H + i\varepsilon)^{-1}V$ .

Let us now return to the unitarity relations (15.168) for the reduced  $T$ -matrix elements, and consider the particular case  $a = b$ . We then have

$$2 \operatorname{Im} T_{aa} = -2\pi \sum_n \delta(E_n - E)\delta(\mathbf{P}_n - \mathbf{P}_a)|T_{na}|^2 \quad (15.171)$$

where  $T_{aa}$  is the reduced transition matrix element for elastic scattering in the forward direction. We may also write this equation as

$$-2\frac{(2\pi)^3}{\hbar v_i} \operatorname{Im} T_{aa} = \frac{(2\pi)^4}{\hbar v_i} \sum_b \delta(E_b - E)\delta(\mathbf{P}_b - \mathbf{P}_a)|T_{ba}|^2 \quad (15.172)$$

where  $v_i$  is the relative initial velocity and we have changed the dummy index of summation from  $n$  to  $b$ . Comparing eq. (15.172) with eq. (15.23) [we recall that  $\hbar = 1$  in eq. (15.23)] and remembering that we sum over *all* final states compatible with energy and momentum conservation, we deduce that the right-hand side of eq. (15.172) is just the *total (complete) cross section* for all processes originating from the initial channel  $a$ .

We shall now transform the left-hand side of eq. (15.172). For a relativistic collision, we see from eq. (15.52) [with  $\phi = \pi$ ] that

$$\operatorname{Im} T_{aa} = -\frac{\hbar^2 c^2}{(2\pi)^2} \frac{E_A + E_B}{E_A E_B} \operatorname{Im} f_{ei}^\circ \quad (15.173)$$

where  $f_{ei}^\circ$  is the forward elastic scattering amplitude and we are working in the C.M. system. In addition, we note from eq. (15.51) that

$$v_i = \hbar c^2 k_i [1/E_A + 1/E_B] \quad (15.174)$$

where  $k_i = |\mathbf{k}_i|$  is the magnitude of the relative initial wave vector. Hence,

$$\operatorname{Im} T_{aa} = -\frac{\hbar v_i}{(2\pi)^2 k_i} \operatorname{Im} f_{ei}^\circ \quad (15.175)$$

We remark that for non-relativistic collisions the result (15.175) may also be obtained directly from eq. (15.54). Indeed, with  $b = a$  and  $M_i = M_r$ , eq. (15.54) yields

$$\text{Im } T_{aa} = - \frac{\hbar^2}{(2\pi)^2 M_i} \text{Im } f_{ei}^\circ = - \frac{\hbar v_i}{(2\pi)^2 k_i} \text{Im } f_{ei}^\circ \quad (15.175')$$

where we have used the fact that  $v_i = \hbar k_i / M_i$  in the non-relativistic case.

Let us now come back to eq. (15.172). Using eq. (15.175) and the fact that the right-hand side of eq. (15.172) is precisely the total cross section  $\sigma_{\text{tot}}$ , we deduce that

$$\sigma_{\text{tot}} = \frac{4\pi}{k_i} \text{Im } f_{ei}^\circ \quad (15.176)$$

which is the (generalized) optical theorem. In the particular case of potential scattering eq. (15.176) reduces to the optical theorem proved in Section 3.4. The more general unitarity relations (15.168) are easily seen to yield the “unitarity relation” (4.94) in the case of scattering by a central potential.

The unitarity relations show in a particularly transparent way that the transition matrix elements corresponding to the various channels of a collision are related. In particular, we see from the generalized optical theorem that *all* the processes (elastic, inelastic, rearrangement) which are allowed at the energy considered – and therefore contribute to the total cross section – also “feed” the imaginary part of the elastic amplitude in the forward direction. In the next chapter we shall obtain a set of equations (the Low equations) which provide even more general relationships between the transition matrix elements than the unitarity relations discussed above.

## References and notes

- [1] It is worth noting that the “box normalization” may be replaced by the “delta function normalization” by taking  $V = (2\pi)^3$ . This is the choice adopted here for the normalization of free waves [see eqs. (5.6)–(5.8)].
- [2] We recall that the index  $\beta$  contains all the information about the momenta and the internal quantum numbers of the particles in the asymptotic region of the final channel.
- [3] Recalling the definition of Section 1.2, we point out that a more precise notation for a given channel  $b$  is  $\bar{b} \equiv (f, \beta')$  where the arrangement channel  $f$  and only the internal quantum numbers  $\beta'$  of the fragments are specified (while  $\beta$  also includes the momenta). In order to simplify the notation we shall not introduce this distinction here.
- [4] The Lorentz–Fitzgerald contraction of a stick moving parallel to its length is the following relativistic effect. Let  $L_0$  be the length of a stick lying along the  $z$  axis and at rest in a reference frame  $O$ . Then, if the reference frame  $O'$  moves with velocity  $u\hat{z}$  with respect to  $O$ , the length  $L$  of the stick in the moving frame  $O'$  may be calculated from the Lorentz transformation (2.64) with the result

$$L = L_0(1 - \beta^2)^{1/2}, \quad \beta = u/c.$$

- [5] MØLLER, C. (1945), Kgl. Danske Videnskab. Selskab., Mat.-fys. Medd. **23**, 1; (1959), *Elementary S matrix Theory* (Nordita, Copenhagen).
- [6] Other definitions of the Lorentz invariant phase space exist, which differ from the one adopted here by numerical factors. For example, one often uses  $dk/[(2\pi)^3 2E]$ .
- [7] More precisely, the matrix elements  $M_{ba}$  are invariant functions when all the particles involved in the collision are spinless. For particles with spin, the *spin averages* of  $M_{ba}$  are invariant.
- [8] We mention here some slightly different definitions of the invariant transition matrix. In our case eqs. (14.174) and (15.83) yield
- $$\langle b|S|a\rangle = \delta_{ba} - 2\pi i \delta^4(P_b - P_a)(E_A E_B E_1 E_2 \dots E_n)^{-\frac{1}{2}} M_{ba}$$
- but some authors define  $M_{ba}$  in such a way that
- $$\langle b|S|a\rangle = \delta_{ba} + i \delta^4(P_b - P_a)(E_A E_B E_1 E_2 \dots E_n)^{-\frac{1}{2}} M_{ba}$$
- or
- $$\langle b|S|a\rangle = \delta_{ba} + i(2\pi)^4 \delta^4(P_b - P_a)[(2\pi)^{3n+6} E_A E_B E_1 E_2 \dots E_n]^{-\frac{1}{2}} M_{ba}, \text{ etc.}$$
- The corresponding cross section formulae are easily established by analogy with the arguments leading to eq. (15.84).
- [9] We note that the choice  $dk/E$  for the one-particle Lips leads to another "normalization" of the plane waves. That is,  $\langle k|k'\rangle = E\delta(k - k')$  and  $\int k \langle k|k\rangle (dk/E) = 1$  so that
- $$\langle r|k\rangle \equiv \Phi_k(r) = (2\pi)^{-3/2} E^{1/2} \exp(ik \cdot r).$$
- [10] The calculation of the phase-space integrals (15.95) or (15.96) is straightforward in the particular case  $n = 2$ , but in the general case these expressions cannot be evaluated in closed form. For a discussion of phase-space integrals and related topics, see for example
- SRIVASTAVA, P. P. and E. C. G. SUDARSHAN (1958), Phys. Rev. **110**, 765;
- HAGEDORN, R. (1966), *Relativistic Kinematics* (Benjamin, New York) Chapter 7;
- LURÇAT, F. and P. MAZUR (1964), Nuovo Cimento **31**, 140;
- KRZYWICKI, A. (1965), J. Math. Phys. **6**, 485;
- PILKUHN, H. (1967), *The Interaction of Hadrons* (North-Holland, Amsterdam) Chapter 1.
- [11] VON NEUMANN, J. (1927), Nachr. Deut. Akad. Wiss. Göttingen, Math.-phys. Kl., 245 and 273.
- [12] FANO, U. (1957), Rev. Mod. Phys. **29**, 74.
- [13] TER HAAR, D. (1961), Theory and Applications of the Density Matrix, in: *Reports on Progress in Physics*, ed. A. C. Strickland (The Physical Society, London) Vol. 24.
- [14] The notion of *statistical ensemble* was introduced in statistical mechanics by Gibbs to replace *time averages* over a single system by ensemble averages, i.e. averages made at a given time over all systems in an ensemble. For a simple introduction to this question, we refer to
- KITTEL, C. (1958), *Elementary Statistical Physics* (Wiley, New York) Chapter 2. A detailed treatment may be found in
- TOLMAN, R. C. (1938), *The Principles of Statistical Mechanics* (Oxford University Press, London) Chapter 9.

## The Determination of the Collision Matrix

We have defined in Chapter 14 the  $S$  and  $T$  matrices and shown in Chapter 15 how the transition probabilities and cross sections may be deduced from the knowledge of the  $T$ -matrix elements. We now attempt to determine the collision matrix  $S$  (or  $T$ ) once the Hamiltonian of the system is known. We begin in Section 16.1 by obtaining the general, multichannel Lippmann–Schwinger equations. The Born series is discussed in Section 16.2, while variational principles of the Schwinger type are given in Section 16.3. In the next section we introduce the Low equations, while in Section 16.5 we discuss the reaction or  $K$  matrix and the Heitler equations. We then generalize in Section 16.6 the considerations developed in Chapter 7 to study collisions involving identical particles. Finally, we analyze in Section 16.7 how invariance principles may be used to simplify the determination of the collision matrix.

### 16.1. The Lippmann–Schwinger equations

Let us return to the important relations (14.66), namely

$$\Psi_a^{(\pm)} = \Phi_a + \frac{1}{E_a - H \pm i\epsilon} V_1 \Phi_a, \quad (16.1a)$$

$$\Psi_b^{(\pm)} = \Phi_b + \frac{1}{E_b - H \pm i\epsilon} V_f \Phi_b \quad (16.1b)$$

and

$$\Psi_n^{(\pm)} = \Phi_n + \frac{1}{E_n - H \pm i\epsilon} V_c \Phi_n. \quad (16.1c)$$

Instead of using the total Green's operators  $G^{(\pm)}(E) = (E - H \pm i\varepsilon)^{-1}$ , let us introduce with the help of eqs. (14.149)–(14.151) the “arrangement channels” Green's operators  $G_c^{(\pm)} = (E - H_c \pm i\varepsilon)^{-1}$ . For example, using eq. (14.150b) we may transform eq. (16.1a) into

$$\begin{aligned}\Psi_a^{(\pm)} &= \Phi_a + \frac{1}{E_a - H_i \pm i\varepsilon} V_i \Phi_a + \frac{1}{E_a - H_i \pm i\varepsilon} V_i \frac{1}{E_a - H \pm i\varepsilon} V_i \Phi_a \\ &= \Phi_a + \frac{1}{E_a - H_i \pm i\varepsilon} V_i \left[ \Phi_a + \frac{1}{E_a - H \pm i\varepsilon} V_i \Phi_a \right].\end{aligned}\quad (16.2)$$

From eq. (16.1a) we see that the quantity in brackets is just  $\Psi_a^{(\pm)}$ , so that

$$\Psi_a^{(\pm)} = \Phi_a + \frac{1}{E_a - H_i \pm i\varepsilon} V_i \Psi_a^{(\pm)}. \quad (16.3a)$$

A similar manipulation using eqs. (16.1b) and (14.151b) yields

$$\Psi_b^{(\pm)} = \Phi_b + \frac{1}{E_b - H_f \pm i\varepsilon} V_f \Psi_b^{(\pm)} \quad (16.3b)$$

while from eqs. (16.1c) and (14.149b)

$$\Psi_n^{(\pm)} = \Phi_n + \frac{1}{E_n - H_c \pm i\varepsilon} V_c \Psi_n^{(\pm)}. \quad (16.3c)$$

The equations (16.3) are known as the *Lippmann–Schwinger* equations. We have obtained them here independently of any choice of representation. They become *integral* equations in the usual representations of quantum theory, for example the position representation  $\{\mathbf{r}\}$  or the momentum representation  $\{\mathbf{p}\}$ . Indeed, in a given representation  $\{\lambda\}$  the relation (16.3a) becomes

$$\langle \lambda | \Psi_a^{(\pm)} \rangle = \langle \lambda | \Phi_a \rangle + \left\langle \lambda \left| \frac{1}{E_a - H_i \pm i\varepsilon} V_i \right| \Psi_a^{(\pm)} \right\rangle. \quad (16.4)$$

If we insert on the right-hand side of eq. (16.4) the completeness relation

$$\sum_{\lambda'} |\lambda'\rangle \langle \lambda'| = I \quad (16.5)$$

we find that

$$\Psi_a^{(\pm)}(\lambda) = \Phi_a(\lambda) + \sum_{\lambda'} \left\langle \lambda \left| \frac{1}{E_a - H_i \pm i\varepsilon} V_i \right| \lambda' \right\rangle \Psi_a^{(\pm)}(\lambda'). \quad (16.6)$$

As an example, let us examine this equation in the position representation  $\{\mathbf{r}\}$  and for the case of non-relativistic potential scattering. Upon using the spectral representation (14.122) of  $(E_a - H_i \pm i\varepsilon)^{-1}$  and the completeness relation (16.5) we have (using the notation of Chapter 5)

$$\begin{aligned}\psi_{k_i}^{(\pm)}(\mathbf{r}) &= \Phi_{k_i}(\mathbf{r}) + \int d\mathbf{r}' d\mathbf{r}'' d\mathbf{k}' \Phi_{k'}(\mathbf{r}) \frac{1}{E_a - E_{k'} \pm i\varepsilon} \Phi_{k'}^*(\mathbf{r}'') \\ &\quad \times \langle \mathbf{r}'' | V | \mathbf{r}' \rangle \psi_{k_i}^{(\pm)}(\mathbf{r}').\end{aligned}\quad (16.7)$$



In particular, for a local potential we have

$$\langle \mathbf{r}'' | V | \mathbf{r}' \rangle = V(\mathbf{r}') \delta(\mathbf{r}'' - \mathbf{r}')$$

so that

$$\psi_{\mathbf{k}_i}^{(\pm)}(\mathbf{r}) = \Phi_{\mathbf{k}_i}(\mathbf{r}) + \int d\mathbf{r}' \int d\mathbf{k}' \Phi_{\mathbf{k}'}(\mathbf{r}) \frac{1}{E_a - E_{\mathbf{k}'} \pm i\varepsilon} \Phi_{\mathbf{k}'}^*(\mathbf{r}') V(\mathbf{r}') \psi_{\mathbf{k}_i}^{(\pm)}(\mathbf{r}'). \quad (16.8)$$

We may now write  $\Phi_{\mathbf{k}'}$  explicitly [see eq. (14.126)] and perform the three-dimensional integral over  $\mathbf{k}'$ . Introducing the reduced potential  $U(\mathbf{r}) = 2mV(\mathbf{r})/\hbar^2$ , we find the familiar Lippmann–Schwinger integral equation for potential scattering

$$\psi_{\mathbf{k}_i}^{(\pm)}(\mathbf{r}) = \Phi_{\mathbf{k}_i}(\mathbf{r}) - \frac{1}{4\pi} \int d\mathbf{r}' \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}') \psi_{\mathbf{k}_i}^{(\pm)}(\mathbf{r}'). \quad (16.9)$$

We have already seen in Chapter 5 that the Lippmann–Schwinger equation (16.9) for two-body (potential) scattering is perfectly well-behaved and has a *unique* solution  $\psi_{\mathbf{k}_i}^{(+)}$  having the asymptotic behaviour

$$\psi_{\mathbf{k}_i}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) + f(\theta, \phi) \frac{e^{ikr}}{r} \right] \quad (16.10a)$$

namely a plane wave of wave vector  $\mathbf{k}_i$  and a spherical *outgoing* wave. Similarly  $\psi_{\mathbf{k}_i}^{(-)}(\mathbf{r})$  is the *unique* solution of eq. (16.9) with the asymptotic behaviour

$$\psi_{\mathbf{k}_i}^{(-)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) + f(\theta, \phi) \frac{e^{-ikr}}{r} \right] \quad (16.10b)$$

corresponding to a plane wave and a spherical *incoming* wave. Therefore the Lippmann–Schwinger equation (16.9) is a “good” integral equation for two-body non-relativistic potential scattering.

Unfortunately, the same nice features are not present when three or more particles are involved. A first difficulty, pointed out by Faddeev [1] in connection with the three-body problem, is that the kernels  $G_i V_i$  or  $G_f V_f$  appearing in eqs. (16.3) are not square integrable ( $\mathcal{L}^2$ ) and cannot be made so by a simple manipulation, as in the case of the two-body problem. We shall examine this point in detail in Section 19.2. Another difficulty, noticed by several authors [2–4] is that the Lippmann–Schwinger equations (16.3) do not have a unique solution when the limit  $\varepsilon \rightarrow 0^+$  is taken before solving the equation. To see this, we shall now show that the *homogeneous* integral equation corresponding to eq. (16.3a) has solutions  $\Psi_m^{(\pm)}$  such that

$$\Psi_m^{(\pm)} = \Phi_m + \frac{1}{E_m - H_i \pm i\varepsilon} V_i \Psi_m^{(\pm)} \quad (16.11)$$

and  $E_m = E_a (m \neq a)$ . Indeed, let us rewrite eq. (16.11) as [see eq. (14.65)]

$$\Psi_m^{(\pm)}(\varepsilon) = \pm i\varepsilon G(E_m \pm i\varepsilon) \Phi_m \quad (16.12)$$

where we have explicitly indicated the dependence on  $\varepsilon$ . Furthermore, using eqs. (14.150b) and (16.12), we find that

$$\Psi_m^{(\pm)}(\varepsilon) = \pm i\varepsilon G_i(E_m \pm i\varepsilon)\Phi_m + G_i(E_m \pm i\varepsilon)V_i\Psi_m^{(\pm)}(\varepsilon). \quad (16.13)$$

Now as  $\varepsilon \rightarrow 0^+$  the first term on the right-hand side of this equation vanishes because  $\Phi_m$  is not an eigenstate of  $H_i$ . Thus, for  $E_m = E_a$ , the quantities  $\Psi_m^{(\pm)}$  are (non-normalizable) solutions of the homogeneous integral equation

$$\Psi^{(\pm)} = G_i^{(\pm)}V_i\Psi^{(\pm)} \quad (16.14)$$

and the Lippmann-Schwinger equation (16.3a) does not have a unique solution. We emphasize that this fact is due to the presence of more than one arrangement channel. In two-body potential scattering it is a simple matter to prove (see Section 5.6) that the homogeneous Lippmann-Schwinger equation has no acceptable solutions in the scattering region.

So far we have discussed the Lippmann-Schwinger equations for the state vectors. We shall now write down similar equations involving the transition operators  $\mathcal{T}_{fi}$  (or  $U_{fi}$ ) and  $\bar{\mathcal{T}}_{fi}$  (or  $\bar{U}_{fi}$ ) defined in Section 14.4. Using eq. (16.1a) together with the identity (14.151b) and the definition (14.155) we first note that

$$\Psi_a^{(+)} = \Phi_a + \frac{1}{E_a - H_f + i\varepsilon} \left[ V_i + V_f \frac{1}{E_a - H + i\varepsilon} V_i \right] \Phi_a$$

or

$$\Psi_a^{(+)} = \Phi_a + \frac{1}{E_a - H_f + i\varepsilon} \mathcal{T}_{fi}(E_a)\Phi_a \quad (16.15)$$

so that we have obtained a formal solution of the Lippmann-Schwinger equation (16.3a) in terms of the operators  $G_f^{(+)}$  and  $\mathcal{T}_{fi}$ . Using the identity (14.151b) together with the definition of  $\mathcal{T}_{fi}$  we observe that the operator  $\mathcal{T}_{fi}$  itself satisfies the Lippmann-Schwinger equation

$$\mathcal{T}_{fi} = V_i + V_f \frac{1}{E - H_f + i\varepsilon} \mathcal{T}_{fi}. \quad (16.16)$$

Similarly, from the definition (14.163) of the operator  $\bar{\mathcal{T}}_{fi}$  and the identity (14.150a) we also find that  $\bar{\mathcal{T}}_{fi}$  satisfies the equation

$$\bar{\mathcal{T}}_{fi} = V_f + \bar{\mathcal{T}}_{fi} \frac{1}{E - H_i + i\varepsilon} V_i. \quad (16.17)$$

In the simple case of a direct collision ( $V_i = V_f = V_d$ ) the transition operator  $\mathcal{T}$  is defined by eq. (14.169). Then, upon using the identities (14.153), we find that  $\mathcal{T}$  satisfies the Lippmann-Schwinger equations

$$\mathcal{T} = V_d + V_d \frac{1}{E - H_d + i\varepsilon} \mathcal{T} \quad (16.18a)$$

and

$$\mathcal{T} = V_d + \mathcal{T} \frac{1}{E - H_d + i\varepsilon} V_d. \quad (16.18b)$$

When  $V_d = V$  (the full interaction between the colliding particles) we shall write

$$\mathcal{T} = V + V \frac{1}{E - H_0 + i\varepsilon} \mathcal{T} \quad (16.19a)$$

and

$$\mathcal{T} = V + \mathcal{T} \frac{1}{E - H_0 + i\varepsilon} V. \quad (16.19b)$$

The various Lippmann–Schwinger equations (16.16)–(16.19) for the transition operators can be replaced by *off-the-energy-shell equations* for the corresponding matrix elements. For example, if we insert a complete set of free states on the right-hand side of eqs. (16.19) and use the definitions (14.171), we find that

$$\langle b | \mathcal{T}^{(+)} | a \rangle = \langle b | V | a \rangle + \sum_n \frac{1}{E_a - E_n + i\varepsilon} \langle b | V | n \rangle \langle n | \mathcal{T}^{(+)} | a \rangle \quad (16.20a)$$

and

$$\langle b | \mathcal{T}^{(-)} | a \rangle = \langle b | V | a \rangle + \sum_n \frac{1}{E_b - E_n + i\varepsilon} \langle b | \mathcal{T}^{(-)} | n \rangle \langle n | V | a \rangle \quad (16.20b)$$

with  $E_a \neq E_b$ . We remark that there is no analogue of eqs. (16.20) for the on-the-energy shell  $T$ -matrix elements  $\langle b | \mathcal{T} | a \rangle$ , since we require the insertion of a complete set of states. The on-shell  $T$ -matrix elements  $\langle b | \mathcal{T} | a \rangle$  must be computed by first obtaining either  $\langle b | \mathcal{T}^{(+)} | a \rangle$  or  $\langle b | \mathcal{T}^{(-)} | a \rangle$  from eqs. (16.20a) or (16.20b) and *then* setting  $E_a = E_b$ . Similar equations may be written down for the completely off-the-energy-shell matrix element  $\langle \Phi_b(E_b) | \mathcal{T}(E) | \Phi_a(E_a) \rangle$ . That is,

$$\begin{aligned} \langle \Phi_b(E_b) | \mathcal{T}(E) | \Phi_a(E_a) \rangle &= \langle \Phi_b(E_b) | V | \Phi_a(E_a) \rangle \\ &+ \sum_n \frac{1}{E - E_n + i\varepsilon} \langle \Phi_b(E_b) | V | \Phi_n(E_n) \rangle \langle \Phi_n(E_n) | \mathcal{T}(E) | \Phi_a(E_a) \rangle \end{aligned} \quad (16.20c)$$

or

$$\begin{aligned} \langle \Phi_b(E_b) | \mathcal{T}(E) | \Phi_a(E_a) \rangle &= \langle \Phi_b(E_b) | V | \Phi_a(E_a) \rangle \\ &+ \sum_n \frac{1}{E - E_n + i\varepsilon} \langle \Phi_b(E_b) | \mathcal{T}(E) | \Phi_n(E_n) \rangle \langle \Phi_n(E_n) | V | \Phi_a(E_a) \rangle. \end{aligned} \quad (16.20d)$$

In order to illustrate these equations on a simple example, let us consider the non-relativistic potential scattering of a spinless particle having a mass  $m$ .

We then write eq. (16.20a) as

$$\langle \mathbf{k}_f | \mathcal{T}^{(+)} | \mathbf{k}_i \rangle = \langle \mathbf{k}_f | V | \mathbf{k}_i \rangle + \int d\mathbf{k}' \frac{\langle \mathbf{k}_f | V | \mathbf{k}' \rangle \langle \mathbf{k}' | \mathcal{T}^{(+)} | \mathbf{k}_i \rangle}{E(k_i) - E(k') + i\epsilon} \quad (16.21a)$$

with  $E(k_i) = \hbar^2 k_i^2 / 2m$ ,  $E(k_f) = \hbar^2 k_f^2 / 2m$ ,  $E(k') = \hbar^2 k'^2 / 2m$  and  $k_i \neq k_f$ . Similarly, eq. (16.20b) yields

$$\langle \mathbf{k}_f | \mathcal{T}^{(-)} | \mathbf{k}_i \rangle = \langle \mathbf{k}_f | V | \mathbf{k}_i \rangle + \int d\mathbf{k}' \frac{\langle \mathbf{k}_f | \mathcal{T}^{(-)} | \mathbf{k}' \rangle \langle \mathbf{k}' | V | \mathbf{k}_i \rangle}{E(k_f) - E(k') + i\epsilon} \quad (16.21b)$$

with  $k_i \neq k_f$ . For the completely off-the-energy-shell  $T$ -matrix element we deduce for example from eq. (16.20c) that

$$\langle \mathbf{k}_f | \mathcal{T}(E) | \mathbf{k}_i \rangle = \langle \mathbf{k}_f | V | \mathbf{k}_i \rangle + \int d\mathbf{k}' \frac{\langle \mathbf{k}_f | V | \mathbf{k}' \rangle \langle \mathbf{k}' | \mathcal{T}(E) | \mathbf{k}_i \rangle}{E(k) - E(k') + i\epsilon} \quad (16.21c)$$

with  $E(k) = \hbar^2 k^2 / 2m$  and  $k \neq k_i \neq k_f$ .

For a spherically symmetric potential it is convenient to analyze the above equations by carrying out the partial wave decompositions:

$$\langle \mathbf{k}_f | V | \mathbf{k}_i \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} V_l(k_f, k_i) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \quad (16.22a)$$

$$\langle \mathbf{k}_f | \mathcal{T}^{(\pm)} | \mathbf{k}_i \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} T_l^{(\pm)}(k_f, k_i) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) \quad (16.22b)$$

and

$$\langle \mathbf{k}_f | \mathcal{T}(E) | \mathbf{k}_i \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} T_l(k_f, k_i, E) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i). \quad (16.22c)$$

We shall also write sometimes the partial wave expression  $T_l(k_f, k_i, E)$  as  $T_l(k_f, k_i, k)$ , (with  $k_i \neq k_f \neq k$ ). We see from the above equations and the definitions (14.171) that

$$T_l^{(+)}(k_f, k_i) = T_l(k_f, k_i, k_i) \quad (16.23a)$$

and

$$T_l^{(-)}(k_f, k_i) = T_l(k_f, k_i, k_f). \quad (16.23b)$$

Furthermore, on the energy shell ( $k_i = k_f = k$ ), we shall write

$$V_l(k) = V_l(k, k) \quad (16.24a)$$

and [5]

$$T_l(k) = T_l^{(\pm)}(k, k). \quad (16.24b)$$

Let us now return to the Lippmann–Schwinger equations (16.21). After performing the partial wave decompositions (16.22) we obtain

$$T_l^{(+)}(k_f, k_i) = V_l(k_f, k_i) + \int_0^{\infty} dk' k'^2 \frac{V_l(k_f, k') T_l^{(+)}(k', k_i)}{E(k_i) - E(k') + i\epsilon} \quad (16.25a)$$

$$T_l^{(-)}(k_f, k_i) = V_l(k_f, k_i) + \int_0^{\infty} dk' k'^2 \frac{T_l^{(-)}(k_f, k') V_l(k', k_i)}{E(k_f) - E(k') + i\epsilon} \quad (16.25b)$$

and

$$T_i(k_f, k_i, k) = V_i(k_f, k_i) + \int_0^\infty dk' k'^2 \frac{V_i(k_f, k')T_i(k', k_i, k)}{E(k) - E(k') + i\epsilon}. \quad (16.25c)$$

The physical (on-the-energy-shell) partial wave  $T$ -matrix is obtained by first solving eq. (16.25a) or (16.25b) and then using eq. (16.24b).

## 16.2. The Born series

Let us attempt to solve the Lippmann–Schwinger equations (16.3) by successive iterations. For example, starting from the “free” states  $\Phi_a$  and  $\Phi_b$ , we find that

$$\Psi_a^{(\pm)} = \Phi_a + G_i^{(\pm)}V_i\Phi_a + G_i^{(\pm)}V_iG_i^{(\pm)}V_i\Phi_a + \dots \quad (16.26a)$$

and

$$\Psi_b^{(\pm)} = \Phi_b + G_f^{(\pm)}V_f\Phi_b + G_f^{(\pm)}V_fG_f^{(\pm)}V_f\Phi_b + \dots \quad (16.26b)$$

which we may call respectively the “prior” and “post” Born series for the state vectors. Another slightly different way of proceeding is to first solve by iteration the Lippmann–Schwinger equations (14.149)–(14.151) for the total Green’s operators. In this way we generate the Born series for  $G^{(\pm)}$ , namely

$$G^{(\pm)} = G_c^{(\pm)} + G_c^{(\pm)}V_cG_c^{(\pm)} + G_c^{(\pm)}V_cG_c^{(\pm)}V_cG_c^{(\pm)} + \dots \quad (16.27a)$$

and in particular

$$G^{(\pm)} = G_i^{(\pm)} + G_i^{(\pm)}V_iG_i^{(\pm)} + G_i^{(\pm)}V_iG_i^{(\pm)}V_iG_i^{(\pm)} + \dots \quad (16.27b)$$

$$G^{(\pm)} = G_f^{(\pm)} + G_f^{(\pm)}V_fG_f^{(\pm)} + G_f^{(\pm)}V_fG_f^{(\pm)}V_fG_f^{(\pm)} + \dots \quad (16.27c)$$

Then, using the formal solutions (16.1) we immediately obtain the developments (16.26), but more generally we also find that

$$\Psi_a^{(\pm)} = \Phi_a + G_c^{(\pm)}V_i\Phi_a + G_c^{(\pm)}V_cG_c^{(\pm)}V_i\Phi_a + \dots \quad (16.28a)$$

and

$$\Psi_b^{(\pm)} = \Phi_b + G_c^{(\pm)}V_f\Phi_b + G_c^{(\pm)}V_cG_c^{(\pm)}V_f\Phi_b + \dots \quad (16.28b)$$

Upon substitution of these expressions in eq. (14.157) we then obtain for the (on the energy shell) transition matrix element  $\langle b|\mathcal{T}|a\rangle$  the Born series

$$\langle b|\mathcal{T}|a\rangle = \langle \Phi_b|V_i(\text{or } V_f) + V_fG_c^{(+)}V_i + V_fG_c^{(+)}V_cG_c^{(+)}V_i + \dots|\Phi_a\rangle. \quad (16.29a)$$

In particular we may write

$$\langle b|\mathcal{T}|a\rangle = \langle \Phi_b|V_i(\text{or } V_f) + V_fG_i^{(+)}V_i + V_fG_i^{(+)}V_iG_i^{(+)}V_i + \dots|\Phi_a\rangle \quad (16.29b)$$

and

$$\langle b|\mathcal{T}|a\rangle = \langle \Phi_b|V_i(\text{or } V_f) + V_fG_f^{(+)}V_i + V_fG_f^{(\pm)}V_fG_f^{(+)}V_i + \dots|\Phi_a\rangle. \quad (16.29c)$$

The first Born approximation consists in retaining only the first term of these expansions, namely

$$\langle b|\mathcal{T}|a\rangle_{B1} = \langle \Phi_b|V_i|\Phi_a\rangle \quad (16.30a)$$

$$= \langle \Phi_b|V_f|\Phi_a\rangle \quad (16.30b)$$

where we have used eq. (14.159) to justify the second equality. The expression  $\langle \Phi_b | V_i | \Phi_a \rangle$  is often called the “prior” form of the (first) Born approximation, while  $\langle \Phi_b | V_f | \Phi_a \rangle$  is denoted as the “post” form. Although formal scattering theory tells us that the two expressions (16.30) are strictly equivalent (on the energy shell), it is worth noting that this equality no longer holds when *approximate* free states  $\Phi_a$  and  $\Phi_b$  are used. For example, a “*post-prior discrepancy*” develops as soon as the bound state wave functions describing the possible internal structure of the colliding systems are not known exactly. This, of course, is the case for almost all collision processes involving composite particles.

Let us return to the Born series (16.29) for the transition matrix element. We note that for *direct* collisions, such that  $V_i = V_f = V_d$ , we may write

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | V_d + V_d G_d^{(+)} V_d + V_d G_d^{(+)} V_d G_d^{(+)} V_d + \cdots | \Phi_a \rangle \quad (16.31)$$

where  $G_d^{(+)} = (E - H_d + i\epsilon)^{-1}$  and  $H_d = H_i = H_f = H - V_d$ . It is also clear that formulae entirely similar to those obtained above may be written down for the *reduced*  $T$ -matrix element  $T_{ba}$  on the energy-momentum shell. For example, eq. (16.29a) yields

$$T_{ba} = \langle \Phi_b | V_i (\text{or } V_f) + V_f G_c^{(+)} V_i + V_f G_c^{(+)} V_c G_c^{(+)} V_i + \cdots | \Phi_a \rangle \quad (16.32)$$

and in first Born approximation we shall write

$$T_{ba}^{B1} = \langle \Phi_b | V_f | \Phi_a \rangle = \langle \Phi_b | V_i | \Phi_a \rangle. \quad (16.33)$$

These matrix elements obviously depend on the total momentum  $\mathbf{P} = \mathbf{P}_a = \mathbf{P}_b$  in a way which is influenced by our choice of coordinate system. In the center of mass framework, where  $\mathbf{P} = 0$ , we simply omit the variables of translation in  $\Phi_a$  and  $\Phi_b$ .

Little is known about the mathematical properties of the general Born series (16.29). For *direct collisions* (no rearrangements) the conditions of convergence of the series (16.31) are probably similar to those discussed in Section 8.4 for the simple case of non-relativistic potential scattering. For example, the Born series (16.31) may well be convergent for non-relativistic direct processes at sufficiently high colliding energies. We shall return to this question in Sections 19.5 and 21.1. In particular, we shall see in the case of the non-relativistic *elastic* scattering of charged particles (electrons) by atoms (hydrogen and helium) that the *first Born* approximation eventually governs the scattering at sufficiently high energies. For *inelastic* (direct) collisions of charged particles by atoms the *two first* terms of the Born series dominate the scattering at high (non-relativistic) energies.

On the other hand, for *rearrangement collisions* some particles are transferred between the colliding systems during the reaction, so that  $V_i \neq V_f$  and the more general series (16.29) must be considered. The question of the convergence of the Born series (16.29) has been investigated by several

authors [6–11]. At low energies the series diverges because the potentials are strong enough to bind particles. At *high energies*, Dettmann and Leibfried [10] have shown that for non-relativistic rearrangement processes occurring in three-body systems the energy variation of the  $T$ -matrix element is given correctly by the *two* first terms of the Born series.

### 16.3. Variational principles

In this section we shall derive variational principles of the Schwinger type which generalize the expressions obtained in Section 10.2 for potential scattering [2, 12, 13]. The application of the Hulthén–Kohn principle to a particular three-body problem (electron–atomic hydrogen scattering) will be discussed in Section 19.5.

We begin by recalling eqs. (14.53), namely

$$\Psi_a^{(\pm)} = \Omega_i^{(\pm)} \Phi_a \quad (16.34a)$$

and

$$\Psi_b^{(\pm)} = \Omega_f^{(\pm)} \Phi_b \quad (16.34b)$$

where the Møller wave operators are given in terms of the full Green's operators  $G^{(\pm)}$  as

$$\Omega_i^{(\pm)} = 1 + G^{(\pm)} V_i \quad (16.35a)$$

and

$$\Omega_f^{(\pm)} = 1 + G^{(\pm)} V_f. \quad (16.35b)$$

Comparing eqs. (16.35) and using the fact that  $G^{(\mp)\dagger} = G^{(\pm)}$ , we find that

$$V_f [\Omega_i^{(+)} - 1] = [\Omega_f^{(-)} - 1]^\dagger V_i. \quad (16.36)$$

Furthermore, by using eqs. (14.150b) and (14.151b), we obtain from eqs. (16.35) the relations

$$(1 - G_i^{(\pm)} V_i) \Omega_i^{(\pm)} = 1 \quad (16.37a)$$

and

$$(1 - G_f^{(\pm)} V_f) \Omega_f^{(\pm)} = 1 \quad (16.37b)$$

from which one readily deduces that

$$(1 - G_f^{(+)} V_f) (\Omega_i^{(+)} - 1) = G_f^{(+)} V_i, \quad (16.38a)$$

$$(\Omega_f^{(-)} - 1)^\dagger (1 - V_i G_i^{(+)} ) = V_f G_i^{(+)}, \quad (16.38b)$$

$$\Omega_f^{(-)\dagger} (V_f - V_f G_f^{(+)} V_f) (\Omega_i^{(+)} - 1) = \Omega_f^{(-)\dagger} V_f G_f^{(+)} V_i \quad (16.38c)$$

and

$$(\Omega_f^{(-)} - 1)^\dagger (V_i - V_i G_i^{(+)} V_i) \Omega_i^{(+)} = V_f G_i^{(+)} V_i \Omega_i^{(+)}. \quad (16.38d)$$

Let us now consider the transition operator (14.163). Using eq. (16.35a) we may write it as

$$\bar{\mathcal{T}}_{fi} = V_f \Omega_i^{(+)} \quad (16.39)$$

or, by using the identity (16.36),

$$\bar{\mathcal{T}}_{fi} = \Omega_f^{(-)\dagger} V_i + (V_f - V_i). \quad (16.40)$$

After these preparations, we shall now establish a pair of variational principles for  $\bar{\mathcal{T}}_{fi}$ . Consider the expression

$$[R_1] = \Omega_f^{(-)\dagger} V_f G_f^{(+)} V_i + V_f \Omega_i^{(+)} - \Omega_f^{(-)\dagger} (V_f - V_i G_f^{(+)} V_f) (\Omega_i^{(+)} - 1). \quad (16.41)$$

Using eqs. (16.38c) and (16.39) we note that its exact value is just

$$[R_1] = \bar{\mathcal{T}}_{fi}. \quad (16.42)$$

Moreover, this expression is stationary for independent variations of the Møller wave operators about their correct values. Indeed,

$$\begin{aligned} \delta[R_1] = & \delta \Omega_f^{(-)\dagger} V_f \{ G_f^{(+)} V_i - (1 - G_f^{(+)} V_f) (\Omega_i^{(+)} - 1) \} \\ & + \{ 1 - \Omega_f^{(-)\dagger} (1 - V_f G_f^{(+)} V_f) \} V_f \delta \Omega_i^{(+)} \end{aligned} \quad (16.43)$$

so that from eqs. (16.37b) and (16.38a) we deduce that

$$\delta[R_1] = 0. \quad (16.44)$$

Therefore the expression (16.41) provides a *variational principle* for the operator  $\bar{\mathcal{T}}_{fi}$ . Since it only uses the Green's operator  $G_f^{(+)}$  we shall call it the "post" form.

A corresponding "prior" variational principle, using the Green's operator  $G_i^{(+)}$  is given by

$$\begin{aligned} [R_2] = & V_f G_i^{(+)} V_i \Omega_i^{(+)} + \Omega_f^{(-)\dagger} V_i + (V_f - V_i) \\ & - (\Omega_f^{(-)} - 1)^\dagger (V_i - V_i G_i^{(+)} V_i) \Omega_i^{(+)}. \end{aligned} \quad (16.45)$$

Indeed, using the relations (16.38d) and (16.40), we have

$$[R_2] = \bar{\mathcal{T}}_{fi} \quad (16.46)$$

while, from the identities (16.37a) and (16.38b), we deduce that

$$\delta[R_2] = 0. \quad (16.47)$$

We may obtain *bilinear forms* of these variational principles by taking the matrix elements of the stationary expressions  $[R_1]$  and  $[R_2]$  between the free states  $\Phi_a$  and  $\Phi_b$  (see Section 10.2). Remembering that the (on the energy shell) transition matrix element  $\langle b | \mathcal{T} | a \rangle$  is given by

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | \bar{\mathcal{T}}_{fi} | \Phi_a \rangle \quad (16.48)$$

and dealing directly with the reduced  $T$ -matrix elements  $T_{ba}$ , we find for  $T_{ba}$  the following "post" stationary expression

$$\begin{aligned} [T_{ba}] = & \langle \Psi_b^{(-)} | V_f \{ 1 + G_f^{(+)} (V_i - V_f) \} | \Phi_a \rangle \\ & + \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle - \langle \Psi_b^{(-)} | V_f - V_f G_f^{(+)} V_f | \Psi_a^{(+)} \rangle \end{aligned} \quad (16.49a)$$



where we have used eqs. (16.34). Similarly, the “prior” form is given by

$$[T_{ba}] = \langle \Phi_b | \{1 + (V_f - V_i)G_i^{(+)}\} V_i | \Psi_a^{(+)} \rangle \\ + \langle \Psi_b^{(-)} | V_i | \Phi_a \rangle - \langle \Psi_b^{(-)} | V_i - V_i G_i^{(+)} V_i | \Psi_a^{(+)} \rangle. \quad (16.49b)$$

Finally, the *fractional* form of the variational principles is obtained by substituting

$$\Psi_a^{(+)} \rightarrow A \Psi_a^{(+)}, \quad \Psi_b^{(-)} \rightarrow B \Psi_b^{(-)}, \quad (16.50)$$

in eqs. (16.49) and treating the coefficients  $A$  and  $B$  as variational parameters. That is, we use the equations

$$\frac{\partial}{\partial A}[T_{ba}] = 0, \quad \frac{\partial}{\partial B}[T_{ba}] = 0 \quad (16.51)$$

to determine  $A$  and  $B$ . We then return to eqs. (16.49) which yield respectively the fractional “post” form

$$[T_{ba}] = \frac{\langle \Phi_b | V_f | \Psi_a^{(+)} \rangle \langle \Psi_b^{(-)} | V_f \{1 + G_f^{(+)}(V_i - V_f)\} | \Phi_a \rangle}{\langle \Psi_b^{(-)} | V_f - V_f G_f^{(+)} V_f | \Psi_a^{(+)} \rangle} \quad (16.52a)$$

and the fractional “prior” form

$$[T_{ba}] = \frac{\langle \Psi_b^{(-)} | V_i | \Phi_a \rangle \langle \Phi_b | \{1 + (V_f - V_i)G_i^{(+)}\} V_i | \Psi_a^{(+)} \rangle}{\langle \Psi_b^{(-)} | V_i - V_i G_i^{(+)} V_i | \Psi_a^{(+)} \rangle}. \quad (16.52b)$$

We note that the bilinear and fractional variational principles obtained above reduce to the expressions derived in Section 10.2 in the particular case of *direct* collisions ( $V_i = V_f = V_d$ ).

It is also worth noting that if in the fractional expressions (16.52) we replace in first approximation the unknown state vectors  $\Psi_a^{(+)}$  and  $\Psi_b^{(-)}$  by the Born “free” states  $\Phi_a$  and  $\Phi_b$  we obtain the following approximate expressions

$$[T_{ba}] \simeq T_{ba}^{B1} \left[ 1 + \frac{\langle \Phi_b | V_f G_f^{(+)} V_i | \Phi_a \rangle}{\langle \Phi_b | V_f - V_f G_f^{(+)} V_f | \Phi_a \rangle} \right] \quad (16.53a)$$

or

$$[T_{ba}] \simeq T_{ba}^{B1} \left[ 1 + \frac{\langle \Phi_b | V_f G_i^{(+)} V_i | \Phi_a \rangle}{\langle \Phi_b | V_i - V_i G_i^{(+)} V_i | \Phi_a \rangle} \right] \quad (16.53b)$$

where  $T_{ba}^{B1}$  is the first Born approximation to the transition matrix element [see eq. (16.33)]. We see that if we neglect the entire second term in the bracket we recover the first Born approximation. On the other hand, if we neglect the “second order” part of the denominators we find the second Born expressions

$$T_{ba}^{B2}(\text{post}) = T_{ba}^{B1} + \langle \Phi_b | V_f G_f^{(+)} V_i | \Phi_a \rangle \quad (16.54a)$$

and

$$T_{ba}^{B2}(\text{prior}) = T_{ba}^{B1} + \langle \Phi_b | V_i G_i^{(+)} V_i | \Phi_a \rangle. \quad (16.54b)$$

We remark that even in its simplified form (16.53) the Schwinger variational principle involves the evaluation of complicated second order terms. We also note that since the variational principles obtained above are not in general minimum principles, the expressions (16.53) do not necessarily yield more accurate results than the first or second Born approximations. We recall in this connection [see the discussion following eqs. (10.67)–(10.69)] that difficulties can arise when poor trial functions are used in variational principles.

### 16.4. The Low equations

Let us start from the *off-shell* matrix elements  $\langle b|\mathcal{T}^{(+)}|a\rangle$  and  $\langle b|\mathcal{T}^{(-)}|a\rangle$  defined by eqs. (14.162). Using eqs. (14.155) and (14.163), we write

$$\langle b|\mathcal{T}^{(+)}|a\rangle = \left\langle \Phi_b(E_b) \left| V_f + V_f \frac{1}{E_a - H + i\varepsilon} V_i \right| \Phi_a(E_a) \right\rangle \quad (16.55a)$$

and

$$\langle b|\mathcal{T}^{(-)}|a\rangle = \left\langle \Phi_b(E_b) \left| V_i + V_i \frac{1}{E_b - H + i\varepsilon} V_f \right| \Phi_a(E_a) \right\rangle. \quad (16.55b)$$

We now introduce a complete set of states  $\{\Psi_n^{(\pm)}, \Psi^{(B)}\}$  which are eigenstates of the total Hamiltonian  $H$ , with  $\Psi_n^{(\pm)}$  corresponding to the continuum part of the spectrum and  $\Psi^{(B)}$  to the bound states [14]. Thus [see eq. (14.41)]

$$\sum_n |\Psi_n^{(+)}\rangle\langle\Psi_n^{(+)}| + \sum_B |\Psi^{(B)}\rangle\langle\Psi^{(B)}| = I \quad (16.56a)$$

and

$$\sum_n |\Psi_n^{(-)}\rangle\langle\Psi_n^{(-)}| + \sum_B |\Psi^{(B)}\rangle\langle\Psi^{(B)}| = I \quad (16.56b)$$

where the summation over the index  $n$  contains integrations over continuous variables. Using eq. (16.56a) in eq. (16.55a), we then obtain

$$\begin{aligned} \langle b|\mathcal{T}^{(+)}|a\rangle &= \langle \Phi_b|V_f|\Phi_a\rangle + \sum_n \langle \Phi_b|V_f|\Psi_n^{(+)}\rangle \left\langle \Psi_n^{(+)} \left| \frac{1}{E_a - H + i\varepsilon} V_i \right| \Phi_a \right\rangle \\ &\quad + \sum_B \langle \Phi_b|V_f|\Psi^{(B)}\rangle \left\langle \Psi^{(B)} \left| \frac{1}{E_a - H + i\varepsilon} V_i \right| \Phi_a \right\rangle. \end{aligned} \quad (16.57)$$

But

$$\langle \Phi_b|V_f|\Psi_n^{(+)}\rangle = \langle b|\mathcal{T}^{(+)}|n\rangle \quad (16.58)$$

and

$$\begin{aligned} \left\langle \Psi_n^{(+)} \left| \frac{1}{E_a - H + i\varepsilon} V_i \right| \Phi_a \right\rangle &= \frac{1}{E_a - E_n + i\varepsilon} \langle \Psi_n^{(+)}|V_i|\Phi_a\rangle \\ &= \frac{1}{E_a - E_n + i\varepsilon} \langle a|\mathcal{T}^{(+)}|n\rangle^* \end{aligned} \quad (16.59)$$

where we have used the hermiticity of the operators  $H$  and  $V_i$ . We also find that

$$\left\langle \Psi^{(B)} \left| \frac{1}{E_a - H + i\varepsilon} V_i \right| \Phi_a \right\rangle = \frac{1}{E_a - E_B} \langle \Psi^{(B)} | V_i | \Phi_a \rangle \quad (16.60)$$

where we have omitted  $\varepsilon$  on the right-hand side because  $E_a \neq E_B$ . Using eqs. (16.58)–(16.60) we rewrite eq. (16.57) as

$$\begin{aligned} \langle b | \mathcal{T}^{(+)} | a \rangle &= \langle \Phi_b | V_i | \Phi_a \rangle + \sum_n \frac{\langle b | \mathcal{T}^{(+)} | n \rangle \langle a | \mathcal{T}^{(+)} | n \rangle^*}{E_a - E_n + i\varepsilon} \\ &\quad + \sum_B \frac{\langle \Phi_b | V_i | \Psi^{(B)} \rangle \langle \Psi^{(B)} | V_i | \Phi_a \rangle}{E_a - E_B}. \end{aligned} \quad (16.61a)$$

In a similar way, we obtain the corresponding equation for  $\langle b | \mathcal{T}^{(-)} | a \rangle$ , namely

$$\begin{aligned} \langle b | \mathcal{T}^{(-)} | a \rangle &= \langle \Phi_b | V_i | \Phi_a \rangle + \sum_n \frac{\langle n | \mathcal{T}^{(-)} | b \rangle^* \langle n | \mathcal{T}^{(-)} | a \rangle}{E_b - E_n + i\varepsilon} \\ &\quad + \sum_B \frac{\langle \Phi_b | V_i | \Psi^{(B)} \rangle \langle \Psi^{(B)} | V_i | \Phi_a \rangle}{E_b - E_B}. \end{aligned} \quad (16.61b)$$

We note that in contrast with the Lippmann–Schwinger equations studied in Section 16.1, the equations (16.61) are no longer linear in the  $T$ -matrix elements.

Since we have

$$\langle \Psi^{(B)} | V_i | \Phi_a \rangle = \langle \Psi^{(B)} | H - H_i | \Phi_a \rangle = (E_B - E_a) \langle \Psi^{(B)} | \Phi_a \rangle \quad (16.62)$$

and similarly

$$\langle \Phi_b | V_i | \Psi^{(B)} \rangle = (E_B - E_b) \langle \Phi_b | \Psi^{(B)} \rangle \quad (16.63)$$

we may rewrite eqs. (16.61) as

$$\begin{aligned} \langle b | \mathcal{T}^{(+)} | a \rangle &= \langle \Phi_b | V_i | \Phi_a \rangle + \sum_n \frac{\langle b | \mathcal{T}^{(+)} | n \rangle \langle a | \mathcal{T}^{(+)} | n \rangle^*}{E_a - E_n + i\varepsilon} \\ &\quad - \sum_B (E_B - E_b) \langle \Phi_b | \Psi^{(B)} \rangle \langle \Psi^{(B)} | \Phi_a \rangle \end{aligned} \quad (16.64a)$$

and

$$\begin{aligned} \langle b | \mathcal{T}^{(-)} | a \rangle &= \langle \Phi_b | V_i | \Phi_a \rangle + \sum_n \frac{\langle n | \mathcal{T}^{(-)} | b \rangle^* \langle n | \mathcal{T}^{(-)} | a \rangle}{E_b - E_n + i\varepsilon} \\ &\quad - \sum_B (E_B - E_a) \langle \Phi_b | \Psi^{(B)} \rangle \langle \Psi^{(B)} | \Phi_a \rangle. \end{aligned} \quad (16.64b)$$

Let us now consider eq. (16.64a). Changing  $b \rightarrow a$ ,  $a \rightarrow b$  and taking the complex conjugate we obtain

$$\begin{aligned} \langle a | \mathcal{T}^{(+)} | b \rangle^* &= \langle \Phi_a | V_i | \Phi_b \rangle^* + \sum_n \frac{\langle a | \mathcal{T}^{(+)} | n \rangle^* \langle b | \mathcal{T}^{(+)} | n \rangle}{E_b - E_n - i\varepsilon} \\ &\quad - \sum_B (E_B - E_a) \langle \Phi_b | \Psi^{(B)} \rangle \langle \Psi^{(B)} | \Phi_a \rangle. \end{aligned} \quad (16.65)$$

Subtracting eq. (16.65) from eq. (16.64a) we then have

$$\begin{aligned} \langle b|\mathcal{T}^{(+)}|a\rangle - \langle a|\mathcal{T}^{(+)}|b\rangle^* &= \sum_n \left( \frac{1}{E_a - E_n + i\varepsilon} - \frac{1}{E_b - E_n - i\varepsilon} \right) \\ &\times \langle b|\mathcal{T}^{(+)}|n\rangle \langle a|\mathcal{T}^{(+)}|n\rangle^* + (E_b - E_a) \sum_B \langle \Phi_b|\Psi^{(B)}\rangle \langle \Psi^{(B)}|\Phi_a\rangle. \end{aligned} \quad (16.66a)$$

Similarly,

$$\begin{aligned} \langle b|\mathcal{T}^{(-)}|a\rangle - \langle a|\mathcal{T}^{(-)}|b\rangle^* &= \sum_n \left( \frac{1}{E_b - E_n + i\varepsilon} - \frac{1}{E_a - E_n - i\varepsilon} \right) \\ &\times \langle n|\mathcal{T}^{(-)}|b\rangle^* \langle n|\mathcal{T}^{(-)}|a\rangle + (E_a - E_b) \sum_B \langle \Phi_b|\Psi^{(B)}\rangle \langle \Psi^{(B)}|\Phi_a\rangle. \end{aligned} \quad (16.66b)$$

The non-linear equations (16.66) for the  $T$ -matrix elements (off-the-energy-shell) are called the *Low equations* [15]. We note that the Low equations reduce to the *unitarity relations* (15.167) *on the energy shell*. Indeed, from the identity (11.167) we deduce that for  $E_a = E_b = E$

$$\frac{1}{E - E_n + i\varepsilon} - \frac{1}{E - E_n - i\varepsilon} = -2\pi i \delta(E - E_n). \quad (16.67)$$

Therefore, using the fact that  $\langle b|\mathcal{T}^{(+)}|a\rangle = \langle b|\mathcal{T}|a\rangle$  on the energy shell we find from eq. (16.66a) that

$$i\{\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*\} = 2\pi \sum_n \delta(E - E_n) \langle b|\mathcal{T}|n\rangle \langle a|\mathcal{T}|n\rangle^* \quad (16.68)$$

which is the unitarity relation (15.167a). We have seen in Section 15.6 that the *optical theorem* is a particular case of eqs. (15.167).

The Low equations (16.66) may be considered as a system of *self-consistent equations* for the  $T$ -matrix elements. They are very general and may be used with little modifications in quantum field theory. Unfortunately, these equations are in most cases extremely difficult to solve. Firstly, all the bound state wave functions must be determined. Then, we need all the off-shell  $T$ -matrix elements, including those between the state  $a$  (or  $b$ ) and bound states.

In certain physical situations, however, one may insert on the right-hand side of eqs. (16.66) a group of intermediate states  $n$  which for physical reasons are believed to be important, and whose  $T$  matrix elements are known. An example of this situation is provided by the Chew and Low model of low-energy pion-nucleon scattering [16].

### 16.5. The reaction matrix and the Heitler integral equations

Since its original introduction by Heitler [17] to analyze radiation damping phenomena, the reaction or  $K$ -matrix (also called the  $R$ -matrix) has been widely used to investigate a variety of quantum collision processes. Of

particular importance is the case of nuclear reactions where the  $R$ -matrix theory was first proposed by Wigner [18, 19] and developed by many others. We list at the end of this chapter a few important references [20–22].

We have already studied above the properties of the solutions  $\Psi_a^{(\pm)}$  or  $\Psi_b^{(\pm)}$  of the Lippmann–Schwinger equations (16.3), which exhibit in configuration space an outgoing (+) or incoming (–) wave behaviour. We shall now be interested in other solutions  $\Psi_a^{(p)}$  and  $\Psi_b^{(p)}$  of the Schrödinger equation, corresponding to different boundary conditions. Indeed, let us define

$$\Psi_a^{(p)} = \Phi_a + \frac{1}{2} \left( \frac{1}{E_a - H_0 + i\varepsilon} + \frac{1}{E_a - H_0 - i\varepsilon} \right) V \Psi_a^{(p)} \quad (16.69a)$$

and

$$\Psi_b^{(p)} = \Phi_b + \frac{1}{2} \left( \frac{1}{E_b - H_0 + i\varepsilon} + \frac{1}{E_b - H_0 - i\varepsilon} \right) V \Psi_b^{(p)} \quad (16.69b)$$

where we have assumed for simplicity that the total Hamiltonian  $H$  may only be split in one way as  $H = H_0 + V$ . By using the identity (11.167), we find that

$$\Psi_a^{(p)} = \Phi_a + P \frac{1}{E_a - H_0} V \Psi_a^{(p)} \quad (16.70a)$$

and

$$\Psi_b^{(p)} = \Phi_b + P \frac{1}{E_b - H_0} V \Psi_b^{(p)} \quad (16.70b)$$

where the symbol

$$P \frac{1}{E - H_0} = \frac{1}{2} \lim_{\varepsilon \rightarrow 0^+} \left( \frac{1}{E - H_0 + i\varepsilon} + \frac{1}{E - H_0 - i\varepsilon} \right) \quad (16.71)$$

means that we have to take the Cauchy principal value when integrating over the continuous spectrum of  $H_0$ . Thus

$$P \frac{1}{E_a - H_0} = P \sum_n \frac{|\Phi_n\rangle \langle \Phi_n|}{E_a - E_n} \quad (16.72)$$

with

$$H_0 \Phi_n = E_n \Phi_n. \quad (16.73)$$

It is clear from eqs. (16.69) that the objects  $\Psi_a^{(p)}$  and  $\Psi_b^{(p)}$  are *standing wave* eigenstates of the Hamiltonian  $H$ . For example, in the case of potential scattering eq. (16.69a) becomes in the coordinate representation

$$\Psi_{k_1}^{(p)}(\mathbf{r}) = \Phi_{k_1}(\mathbf{r}) - \frac{1}{4\pi} \int \frac{\cos(k|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}') \Psi_{k_1}^{(p)}(\mathbf{r}') d\mathbf{r}'. \quad (16.74)$$

Hence, when  $r \rightarrow \infty$ , the wave  $\Psi_{k_1}^{(p)}(\mathbf{r})$  tends towards the plane wave  $\Phi_{k_1}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_1 \cdot \mathbf{r})$ , plus a standing wave whose amplitude is inversely proportional to  $r$ .

Let us now establish the relationship between the objects  $\Psi_a^{(+)}$  and  $\Psi_a^{(P)}$ . From eqs. (16.3a) and (16.70a) we see that

$$\Psi_a^{(+)} - \Psi_a^{(P)} = \frac{1}{E_a - H_0 + i\varepsilon} V \Psi_a^{(+)} - P \frac{1}{E_a - H_0} V \Psi_a^{(P)} \quad (16.75)$$

or, using the identity (11.167),

$$\Psi_a^{(+)} - \Psi_a^{(P)} = P \frac{1}{E_a - H_0} V (\Psi_a^{(+)} - \Psi_a^{(P)}) - i\pi \delta(E_a - H_0) V \Psi_a^{(+)}. \quad (16.76)$$

Introducing a complete set of unperturbed states on the right-hand side of eq. (16.76) between  $\delta(E_a - H_0)$  and  $V \Psi_a^{(+)}$ , and using eq. (14.157), we also have

$$\begin{aligned} \Psi_a^{(+)} - \Psi_a^{(P)} = P \frac{1}{E_a - H_0} V (\Psi_a^{(+)} - \Psi_a^{(P)}) \\ - i\pi \sum_n \delta(E_a - E_n) \langle n | \mathcal{T} | a \rangle \Phi_n. \end{aligned} \quad (16.77)$$

Since the delta function in the summation imposes  $E_n = E_a$ , all the states  $\Phi_n$  belong to the continuum and may be expressed in terms of  $\Psi_n^{(P)}$  by means of eq. (16.70a). Thus

$$\begin{aligned} \Psi_a^{(+)} - \Psi_a^{(P)} = P \frac{1}{E_a - H_0} V (\Psi_a^{(+)} - \Psi_a^{(P)}) - i\pi \sum_n \delta(E_a - E_n) \langle n | \mathcal{T} | a \rangle \\ \times \left( \Psi_n^{(P)} - P \frac{1}{E_n - H_0} V \Psi_n^{(P)} \right) \end{aligned} \quad (16.78)$$

or

$$\begin{aligned} \Psi_a^{(+)} - \Psi_a^{(P)} = P \frac{1}{E_a - H_0} V [\Psi_a^{(+)} - \Psi_a^{(P)} + i\pi \sum_n \delta(E_a - E_n) \langle n | \mathcal{T} | a \rangle \Psi_n^{(P)}] \\ - i\pi \sum_n \delta(E_a - E_n) \langle n | \mathcal{T} | a \rangle \Psi_n^{(P)}. \end{aligned} \quad (16.79)$$

If we set

$$\hat{\Psi} = \Psi_a^{(+)} - \Psi_a^{(P)} + i\pi \sum_n \delta(E_a - E_n) \langle n | \mathcal{T} | a \rangle \Psi_n^{(P)} \quad (16.80)$$

we see that eq. (16.79) is of the form

$$\hat{\Psi} = P \frac{1}{E_a - H_0} V \hat{\Psi}. \quad (16.81)$$

In the simple case which we are considering (one arrangement channel [23]) the only solution  $\hat{\Psi}$  of the homogeneous equation (16.81) which belongs to the continuum is the trivial one  $\hat{\Psi} = 0$ . Hence

$$\Psi_a^{(+)} = \Psi_a^{(P)} - i\pi \sum_n \delta(E_a - E_n) \langle n | \mathcal{T} | a \rangle \Psi_n^{(P)} \quad (16.82a)$$

is the desired relation between  $\Psi_a^{(+)}$  and  $\Psi_a^{(P)}$ . Similarly, we also find that

$$\Psi_b^{(-)} = \Psi_b^{(P)} + i\pi \sum_n \delta(E_b - E_n) \langle b | \mathcal{T} | n \rangle^* \Psi_n^{(P)}. \quad (16.82b)$$

Having studied the standing wave eigenstates  $\Psi_a^{(P)}$  and  $\Psi_b^{(P)}$  of the Hamiltonian  $H$ , we now introduce the  $K$ -matrix elements as follows. We first define *on the energy shell*  $E = E_a = E_b$  the matrix elements

$$\langle b|K|a\rangle = \langle \Phi_b|V|\Psi_a^{(P)}\rangle \quad (16.83a)$$

and we also note that

$$\langle b|K|a\rangle = \langle \Psi_b^{(P)}|V|\Phi_a\rangle. \quad (16.83b)$$

Indeed, using eqs. (16.70), we may write on the energy shell

$$\begin{aligned} \langle b|K|a\rangle &= \langle \Phi_b|V|\Psi_a^{(P)}\rangle \\ &= \langle \Psi_b^{(P)}|V|\Psi_a^{(P)}\rangle - \left\langle \Psi_b^{(P)} \left| V P \frac{1}{E - H_0} V \right| \Psi_a^{(P)} \right\rangle \\ &= \langle \Psi_b^{(P)}|V|\Psi_a^{(P)}\rangle - \langle \Psi_b^{(P)}|V|(\Psi_a^{(P)} - \Phi_a)\rangle \\ &= \langle \Psi_b^{(P)}|V|\Phi_a\rangle, \quad \text{Q.E.D.} \end{aligned}$$

Moreover, we also have

$$\langle b|K|a\rangle^* = \langle \Phi_a|V|\Psi_b^{(P)}\rangle = \langle a|K|b\rangle \quad (16.84)$$

so that the  $K$ -matrix is *Hermitian* on the energy shell.

Let us return to the relations (16.70). They imply that the operator  $K$  whose *on-the-energy shell* matrix elements are given by eqs. (16.83) satisfies the equations

$$K = V + V P \left( \frac{1}{E - H_0} \right) K \quad (16.85a)$$

or

$$K = V + K P \left( \frac{1}{E - H_0} \right) V \quad (16.85b)$$

and is Hermitian, namely

$$K^\dagger = K. \quad (16.86)$$

Natural extensions of the  $K$  matrix off the energy shell may be obtained from eqs. (16.83). Thus we define

$$\langle b|K^{(+)}|a\rangle = \langle \Phi_b(E_b)|V|\Psi_a^{(P)}(E_a)\rangle, \quad E_a \neq E_b \quad (16.87a)$$

and

$$\langle b|K^{(-)}|a\rangle = \langle \Psi_b^{(P)}(E_b)|V|\Phi_a(E_a)\rangle, \quad E_a \neq E_b. \quad (16.87b)$$

Clearly

$$\langle b|K^{(+)}|a\rangle \rightarrow \langle b|K|a\rangle \quad \text{as } E_b \rightarrow E_a, \quad (16.88a)$$

$$\langle b|K^{(-)}|a\rangle \rightarrow \langle b|K|a\rangle \quad \text{as } E_b \rightarrow E_a \quad (16.88b)$$

and we remark that the matrix elements  $\langle b|K^{(+)}|a\rangle$  and  $\langle b|K^{(-)}|a\rangle$  satisfy the *off-the-energy shell* equations [compare with eqs. (16.20)]

$$\langle b|K^{(+)}|a\rangle = \langle b|V|a\rangle + \sum_n P\left(\frac{1}{E_a - E_n}\right) \langle b|V|n\rangle \langle n|K^{(+)}|a\rangle \quad (16.89a)$$

and

$$\langle b|K^{(-)}|a\rangle = \langle b|V|a\rangle + \sum_n P\left(\frac{1}{E_b - E_n}\right) \langle b|K^{(-)}|n\rangle \langle n|V|a\rangle. \quad (16.89b)$$

Moreover, we note that

$$\langle b|K^{(+)}|a\rangle^* = \langle a|K^{(-)}|b\rangle \quad (16.90)$$

an equation which reduces to (16.84) on the energy shell. The *completely off-the-energy shell*  $K$ -matrix elements  $\langle \Phi_b(E_b)|K(E)|\Phi_a(E_a)\rangle$ , where  $E \neq E_a \neq E_b$ , are seen from eqs. (16.85) to satisfy the equation

$$\begin{aligned} \langle \Phi_b(E_b)|K(E)|\Phi_a(E_a)\rangle &= \langle \Phi_b(E_b)|V|\Phi_a(E_a)\rangle \\ &+ \sum_n P\left(\frac{1}{E - E_n}\right) \langle \Phi_b(E_b)|V|\Phi_n(E_n)\rangle \langle \Phi_n(E_n)|K(E)|\Phi_a(E_a)\rangle. \end{aligned} \quad (16.91)$$

The *reduced*  $K$ -matrix elements *on the momentum shell* may be defined by analogy with the corresponding  $T$ -matrix elements [see eqs. (14.174) and (14.175)]. That is,

$$\langle b|K|a\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b) K_{ba}(E), \quad E = E_a = E_b \quad (16.92a)$$

$$\langle b|K^{(\pm)}|a\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b) K_{ba}^{(\pm)}(E_b, E_a), \quad E_b \neq E_a \quad (16.92b)$$

and

$$\langle \Phi_b(E_b)|K(E)|\Phi_a(E_a)\rangle = \delta(\mathbf{P}_a - \mathbf{P}_b) K_{ba}(E_b, E_a, E), \quad E \neq E_a \neq E_b. \quad (16.92c)$$

Let us now return to the relation (16.82a) between  $\Psi_a^{(+)}$  and  $\Psi_a^{(P)}$ . If we operate on both sides of this equation by means of  $\langle \Phi_b|V$ , we obtain (on the energy shell)

$$\langle b|\mathcal{T}|a\rangle = \langle b|K|a\rangle - i\pi \sum_n \delta(E - E_n) \langle b|K|n\rangle \langle n|\mathcal{T}|a\rangle. \quad (16.93a)$$

Similarly, if we rewrite eq. (16.82b) as

$$\langle \Psi_b^{(-)}| = \langle \Psi_b^{(P)}| - i\pi \sum_n \delta(E - E_n) \langle b|\mathcal{T}|n\rangle \langle \Psi_n^{(P)}|$$

and operate on both sides by means of  $V|\Phi_a\rangle$ , we find that

$$\langle b|\mathcal{T}|a\rangle = \langle b|K|a\rangle - i\pi \sum_n \delta(E - E_n) \langle b|\mathcal{T}|n\rangle \langle n|K|a\rangle. \quad (16.93b)$$

The equations (16.93) are known as the *Heitler integral equations* [17]. In terms of the operators  $\mathcal{T}(E)$  and  $K(E)$  we may write

$$\mathcal{T}(E) = K(E) - i\pi K(E)\delta(E - H_0)\mathcal{T}(E) \quad (16.94a)$$

or

$$\mathcal{T}(E) = K(E) - i\pi \mathcal{T}(E)\delta(E - H_0)K(E). \quad (16.94b)$$



An important property of the  $K$  matrix is that *any Hermitian  $K$  matrix which is substituted into the Heitler equations (16.93) leads to a unitary  $S$  matrix.* To see this, we use the Heitler equations to write

$$\begin{aligned} i[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] &= i\langle b|K|a\rangle + \pi \sum_n \delta(E - E_n) \langle b|K|n\rangle \langle n|\mathcal{T}|a\rangle \\ &\quad - i\langle a|K|b\rangle^* + \pi \sum_n \delta(E - E_n) \langle a|K|n\rangle^* \langle n|\mathcal{T}|b\rangle^*. \end{aligned} \quad (16.95)$$

Then, taking into account the fact that  $\langle b|K|a\rangle$  is Hermitian, we have

$$\begin{aligned} i[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] &= \pi \sum_n \delta(E - E_n) [\langle b|K|n\rangle \langle n|\mathcal{T}|a\rangle \\ &\quad + \langle n|K|a\rangle \langle n|\mathcal{T}|b\rangle^*]. \end{aligned} \quad (16.96)$$

Using again the hermiticity of the  $K$  matrix elements and the Heitler equations to modify the right-hand side of eq. (16.96), we find that

$$\begin{aligned} i[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] &= \pi \sum_n \delta(E - E_n) \{ [\langle n|\mathcal{T}|b\rangle^* \\ &\quad - i\pi \sum_{n'} \delta(E - E_{n'}) \langle n|K|n'\rangle^* \langle n'|\mathcal{T}|b\rangle^*] \langle n|\mathcal{T}|a\rangle \\ &\quad + [\langle n|\mathcal{T}|a\rangle + i\pi \sum_{n'} \delta(E - E_{n'}) \langle n|K|n'\rangle \langle n'|\mathcal{T}|a\rangle] \langle n|\mathcal{T}|b\rangle^* \}. \end{aligned} \quad (16.97)$$

Then, after interchanging the indices  $n$  and  $n'$  in the second double sum, we obtain

$$i[\langle b|\mathcal{T}|a\rangle - \langle a|\mathcal{T}|b\rangle^*] = 2\pi \sum_n \delta(E - E_n) \langle n|\mathcal{T}|b\rangle^* \langle n|\mathcal{T}|a\rangle, \quad (16.98)$$

which is precisely the unitarity relation (15.167b). We may also start from the operator equations (16.94) and use the fact that  $K = K^\dagger$  to write

$$\begin{aligned} i(\mathcal{T} - \mathcal{T}^\dagger) &= \pi K \delta(E - H_0) \mathcal{T} + \pi \mathcal{T}^\dagger \delta(E - H_0) K \\ &= \pi [\mathcal{T}^\dagger - i\pi \mathcal{T}^\dagger \delta(E - H_0) K] \delta(E - H_0) \mathcal{T} \\ &\quad + \pi \mathcal{T}^\dagger \delta(E - H_0) [\mathcal{T} + i\pi K \delta(E - H_0) \mathcal{T}] \end{aligned} \quad (16.99)$$

so that

$$i(\mathcal{T} - \mathcal{T}^\dagger) = 2\pi \mathcal{T}^\dagger \delta(E - H_0) \mathcal{T}. \quad (16.100)$$

This result is identical to the operator form (15.170a) of the unitarity relations. The operator form (15.170b) may clearly be obtained in a similar way.

## 16.6. Collisions involving identical particles

In this section we want to investigate the effect of the identity of particles in collision processes, a problem which we already studied in Chapter 7 for the simple case of non-relativistic two-body scattering. We shall now consider more general situations, for example when a particle is incident upon a target containing several scatterers, some of them being identical to the projectile [24]. This is the case for example in electron—atom or nucleon—nucleus scattering.

Let us consider a collision process  $a \rightarrow b$  for which the (unsymmetrized) Lippmann-Schwinger equation (16.3a) reads

$$\Psi_a^{(+)} = \Phi_a + G_i^{(+)} V_i \Psi_a^{(+)} \quad (16.101)$$

where

$$G_i^{(+)} = (E_a - H_i + i\epsilon)^{-1}, \quad H = H_i + V_i, \quad H_i \Phi_a = E_a \Phi_a, \quad (16.102)$$

and  $V_i$  is the interaction potential in the initial channel. The formal solution of eq. (16.101) is given by

$$\Psi_a^{(+)} = \Phi_a + G^{(+)}(E_a) V_i \Phi_a \quad (16.103)$$

with

$$G^{(+)}(E) = (E - H + i\epsilon)^{-1}. \quad (16.104)$$

The free, unsymmetrized, state  $\Phi_a$  is clearly constructed in such a way that it singles out a given particle as the incident one. If we consider for example a system containing  $N = N_0 + 1$  identical particles, of which  $N_0$  are initially bound in a target and one is free, we may write

$$\Phi_a(q_0, q_1, \dots, q_{N_0}) = \psi_\alpha(q_0) \psi_\beta(q_1, \dots, q_{N_0}) \quad (16.105)$$

where  $q_0, q_1, \dots, q_{N_0}$  are the dynamical variables of the particles, and the wave functions  $\psi_\alpha(q_0)$  and  $\psi_\beta(q_1 \dots q_{N_0})$  describe respectively the incident particle and the target. We shall assume in what follows that the target wave function  $\psi_\beta(q_1 \dots q_{N_0})$  has already been properly symmetrized. For example, in the case of an electron having a wave vector  $k_1$  and a spin orientation  $v = +\frac{1}{2}$  incident on a helium atom in the ground state ( $1^1S$ ), the free, unsymmetrized state  $\Phi_a$  is given by

$$\Phi_a = (2\pi)^{-3/2} \exp(ik_1 \cdot r_0) \alpha(0) \psi_{1^1S}(r_1, r_2) \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \alpha(2)\beta(1)]. \quad (16.106)$$

Here the index 0 refers to the “incoming” electron, while the variables 1 and 2 correspond to the “atomic” electrons. The objects  $\alpha$  and  $\beta$  are the spinors

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (16.107)$$

and we have assumed that the nucleus of the helium atom is infinitely heavy.

What we would like to do now is to construct from  $\Phi_a$  a new free state which takes into account properly the identity of the incident and target particles. To this end, we consider the symmetrization operators [24]

$$\mathcal{S}_S = \frac{1}{N!} \sum_P P \quad \text{for bosons (symmetrization)} \quad (16.108a)$$

and

$$\mathcal{S}_A = \frac{1}{N!} \sum_P \epsilon_P P \quad \text{for fermions (antisymmetrization)} \quad (16.108b)$$

where  $P$  is a permutation [25],  $\varepsilon_P = +1$  for an even permutation and  $\varepsilon_P = -1$  for an odd one. The symbol  $\mathcal{A}$  is also often used to denote either  $\mathcal{S}_A$  or the operator  $\sum_P \varepsilon_P P$ . It is a simple matter to show that the operators  $\mathcal{S}_S$  and  $\mathcal{S}_A$  are Hermitian. One also has

$$\mathcal{S}_S^2 = \mathcal{S}_S; \quad \mathcal{S}_A^2 = \mathcal{S}_A \quad (16.109)$$

so that  $\mathcal{S}_S$  and  $\mathcal{S}_A$  are projection operators. Moreover, they commute with the total Hamiltonian for the system of  $N$  identical particles. That is,

$$[\mathcal{S}_S, H] = 0, \quad [\mathcal{S}_A, H] = 0. \quad (16.110)$$

In what follows, we shall often use a single symbol to represent both operators  $\mathcal{S}_A$  and  $\mathcal{S}_S$ . It is defined by

$$\mathcal{S} = \frac{1}{N!} \sum_P \delta_P P \quad (16.111)$$

where  $\delta_P = +1$  for bosons and  $\delta_P = \varepsilon_P$  for fermions.

We are now able to construct an initial free state which is correctly symmetrized. It is given by

$$\bar{\Phi}_a = C \mathcal{S} \Phi_a \quad (16.112)$$

or

$$\bar{\Phi}_a = \frac{C}{N!} \sum_P \delta_P P \Phi_a = \frac{C}{N!} \sum_P \delta_P \Phi_{Pa} \quad (16.113)$$

where  $C$  is a normalization constant and we have set  $\Phi_{Pa} = P\Phi_a$ . If we require the symmetrized state  $\bar{\Phi}_a$  to satisfy the same normalization condition as the unsymmetrized state  $\Phi_a$ , we have

$$\begin{aligned} \langle \bar{\Phi}_a | \bar{\Phi}_a \rangle &= C^2 \langle \Phi_a | \mathcal{S} | \Phi_a \rangle \\ &= \frac{C^2}{N!} \sum_P \delta_P \langle \Phi_a | P | \Phi_a \rangle = \langle \Phi_a | \Phi_a \rangle. \end{aligned} \quad (16.114)$$

Now  $\langle \Phi_a | P | \Phi_a \rangle$  vanishes unless  $P$  belongs to one of the  $N_0!$  permutations of the  $(q_1 \dots q_{N_0})$  variables. Thus, in this case

$$\delta_P \langle \Phi_a | P | \Phi_a \rangle = \langle \Phi_a | \Phi_a \rangle$$

and

$$\frac{C^2}{N!} N_0! = 1$$

so that

$$C = \sqrt{N}. \quad (16.115)$$

The correctly symmetrized free state  $\bar{\Phi}_a$ , corresponding to the unsymmetrized  $\Phi_a$  of eq. (16.105) is thus given by

$$\bar{\Phi}_a = \frac{\sqrt{N}}{N!} \sum_P \delta_P P \psi_\alpha(q_0) \psi_\beta(q_1, \dots, q_{N_0}). \quad (16.116)$$

This expression may be simplified by noting that the  $N!$  permutations  $P$  may be classified into  $N$  types. The first type consists of  $N_0!$  permutations of the variables  $(q_1, \dots, q_{N_0})$  which leave  $\Phi_a$  unchanged since the target wave function  $\psi_\beta$  is already symmetrized with respect to these variables. The remaining  $N_0$  types are obtained by considering the permutations  $P_{0j}$  which interchange  $q_0$  with one of the  $q_j$ 's (with  $j = 1, 2, \dots, N_0$ ). For a given value of  $j$ , there are each time  $N_0!$  permutations of this sort. Furthermore,

$$\delta_{P_{0j}} P_{0j} \Phi_a = \pm \psi_\alpha(q_j) \psi_\beta(q_1, \dots, q_{j-1}, q_0, q_{j+1}, \dots, q_{N_0}) \quad (16.117)$$

with the plus sign for bosons and the minus sign for fermions. Hence we have

$$\bar{\Phi}_a = \frac{\sqrt{N}}{N!} N_0! \sum_{j=0}^{N_0} \delta_j P_{0j} \psi_\alpha(q_0) \psi_\beta(q_1, \dots, q_{N_0}) \quad (16.118)$$

with  $\delta_0 = 1$ ,  $\delta_j = 1$  for bosons and  $\delta_j = -1$  for fermions.

Using eq. (16.105) and the fact that  $N = N_0 + 1$ , we may also write

$$\bar{\Phi}_a = \frac{1}{\sqrt{N}} \sum_{j=0}^{N_0} \delta_j P_{0j} \Phi_a. \quad (16.119)$$

For example, the (anti)symmetrized free state  $\bar{\Phi}_a$  corresponding to the unsymmetrized state (16.106) is given by

$$\begin{aligned} \bar{\Phi}_a = \frac{1}{\sqrt{3}} (1 - P_{01} - P_{02}) & \left\{ (2\pi)^{-3/2} \exp(ik_i \cdot r_0) \alpha(0) \right. \\ & \left. \times \psi_{11s}(r_1, r_2) \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \alpha(2)\beta(1)] \right\} \end{aligned} \quad (16.120)$$

where  $P_{01}$  interchanges the variables "0" and "1" while  $P_{02}$  interchanges those labelled by "0" and "2".

We have analyzed until now the simple case of  $N = N_0 + 1$  identical particles, of which one is initially free and the remaining  $N_0$  ones are bound in the target. More generally we may imagine a system of  $N$  identical "elementary" particles, of which  $n_A$  are initially bound in the "beam" (composite) particle A, while the remaining  $n_B = N - n_A$  particles are contained in the "target" B. In this case the symmetrized state is still given by eq. (16.112), namely

$$\bar{\Phi}_a = C \mathcal{S} \Phi_a = \frac{C}{N!} \sum_P \delta_P P \Phi_a \quad (16.121)$$

but the constant  $C$ , obtained by imposing the normalization condition (16.114) is now given by

$$C = \left[ \frac{N!}{n_A! n_B!} \right]^{1/2}. \quad (16.122)$$

An even more general situation occurs when there are several kinds of elementary particles involved in the collision. This case may be handled by using a straightforward generalization of the symmetrization operators. It will not be analyzed in detail here.

Let us now consider the unsymmetrized state vector  $\Psi_a^{(+)}$ . In order to investigate the action of the permutation operator  $P$  on  $\Psi_a^{(+)}$ , we recast eq. (16.103) in the form [see eq. (14.65)]

$$\Psi_a^{(+)} = i\varepsilon(E_a - H + i\varepsilon)^{-1}\Phi_a. \quad (16.123)$$

Then, since  $[P, H] = 0$ , we have

$$\begin{aligned} P\Psi_a^{(+)} &= i\varepsilon P(E_a - H + i\varepsilon)^{-1}\Phi_a = i\varepsilon(E_a - H + i\varepsilon)^{-1}P\Phi_a \\ &= i\varepsilon(E_a - H + i\varepsilon)^{-1}\Phi_{Pa}. \end{aligned} \quad (16.124)$$

Therefore, if we define the channel Hamiltonian  $H_P$  and the interaction  $V_P$  by the relations

$$H_P\Phi_{Pa} = E_a\Phi_{Pa}, \quad (16.125)$$

$$H_P = PH_1P^{-1} \quad (16.126)$$

and

$$H = H_P + V_P \quad (16.127)$$

we find from eq. (16.124) that

$$\begin{aligned} \Psi_{Pa}^{(+)} &\equiv P\Psi_a^{(+)} = (E_a - H + i\varepsilon)^{-1}(E_a - H_P + i\varepsilon)\Phi_{Pa} \\ &= (E_a - H + i\varepsilon)^{-1}(E_a - H + i\varepsilon + V_P)\Phi_{Pa} \end{aligned}$$

or

$$\Psi_{Pa}^{(+)} = \Phi_{Pa} + G^{(+)}(E_a)V_P\Phi_{Pa}. \quad (16.128)$$

By analogy with our foregoing discussion of the free state, we now define the symmetrized state vector  $\bar{\Psi}_a^{(+)}$  by

$$\bar{\Psi}_a^{(+)} = C\mathcal{S}\Psi_a^{(+)} \quad (16.129)$$

where the symmetrization operator  $\mathcal{S}$  is given by eq. (16.111) and  $C$  is a constant which we determine by the normalization condition (16.114) on the symmetrized initial state  $\bar{\Phi}_a$  [see eq. (16.115) or (16.122)]. We then deduce from eqs. (16.111), (16.128) and (16.129) that

$$\bar{\Psi}_a^{(+)} = \frac{C}{N!} \sum_P \delta_P P\Psi_a^{(+)} = \frac{C}{N!} \sum_P \delta_P \Psi_{Pa}^{(+)} \quad (16.130)$$

or

$$\begin{aligned} \bar{\Psi}_a^{(+)} &= \frac{C}{N!} \sum_P \delta_P [\Phi_{Pa} + G^{(+)}(E_a)V_P\Phi_{Pa}] \\ &= \bar{\Phi}_a + \frac{C}{N!} \sum_P \delta_P G^{(+)}(E_a)V_P\Phi_{Pa}. \end{aligned} \quad (16.131)$$

We have considered so far the symmetrization of the *initial* free state  $\Phi_a$  and of the state vector  $\Psi_a^{(+)}$ . A completely similar procedure may be used to symmetrize the final free state  $\Phi_b$  and the state vector  $\Psi_b^{(-)}$ . Thus we have

$$\bar{\Phi}_b = C'\mathcal{S}\Phi_b = \frac{C'}{(N')!} \sum_{P'} \delta_{P'} \Phi_{P'b} \quad (16.132)$$

where  $P'$  is a permutation among the  $N'$  identical particles in the final state and  $\Phi'_{P'b} = P'\Phi_b$ . The constant  $C'$  is determined by the requirement that

$$\langle \bar{\Phi}_b | \bar{\Phi}_b \rangle = \langle \Phi_b | \Phi_b \rangle \quad (16.133)$$

and we assume that there is only one kind of “elementary” identical particles (the generalization to several kinds of identical “elementary” particles is straightforward). For example, if two composite particles C and D emerge in the final state and contain respectively  $n_C$  and  $n_D = N' - n_C$  “elementary” identical particles, one has

$$C' = \left[ \frac{(N')!}{n_C! n_D!} \right]^{1/2}. \quad (16.134)$$

Furthermore, the object  $\Phi_{P'b}$  appearing in eq. (16.132) is such that

$$H_{P'} \Phi_{P'b} = E_b \Phi_{P'b}, \quad (16.135)$$

with

$$H_{P'} = P' H_f (P')^{-1} \quad (16.136)$$

and we also have

$$H = H_f + V_f \quad (16.137)$$

$$= H_{P'} + V_{P'} \quad (16.138)$$

where  $V_f$  is the final interaction in a given channel  $f$ , corresponding to the unsymmetrized state  $\Phi_b$ . By analogy with eqs. (16.129)–(16.131), we also have

$$\bar{\Psi}_b^{(-)} = C' \mathcal{S} \Psi_b^{(-)} = \frac{C'}{(N')!} \sum_{P'} \delta_{P'} P' \Psi_b^{(-)} \quad (16.139)$$

or

$$\bar{\Psi}_b^{(-)} = \frac{C'}{(N')!} \sum_{P'} \delta_{P'} \Psi_{P'b}^{(-)} \quad (16.140)$$

and

$$\bar{\Psi}_b^{(-)} = \bar{\Phi}_b + \frac{C'}{(N')!} \sum_{P'} \delta_{P'} G^{(-)}(E_b) V_{P'} \Phi_{P'b} \quad (16.141)$$

where we have used the fact that

$$\Psi_{P'b}^{(-)} = P \Psi_b^{(-)} = \Phi_{P'b} + G^{(-)}(E_b) V_{P'} \Phi_{P'b}. \quad (16.142)$$

It is now a simple matter to calculate the  $S$ -matrix element for a general transition between the states  $\bar{\Phi}_a$  and  $\bar{\Phi}_b$ . Using the notation

$$\begin{aligned} |\Phi_{Pa}\rangle &\equiv |Pa\rangle, & |\Phi_{P'b}\rangle &\equiv |P'b\rangle, \\ |\bar{\Phi}_a\rangle &\equiv |\bar{a}\rangle, & |\bar{\Phi}_b\rangle &\equiv |\bar{b}\rangle \end{aligned}$$

and proceeding as in Section 14.2, we find with the help of eqs. (16.131) and (16.141) that the  $S$  matrix element

$$\langle \bar{b} | S | \bar{a} \rangle = \langle \bar{\Psi}_b^{(-)} | \bar{\Psi}_a^{(+)} \rangle \quad (16.143)$$

is given by

$$\langle \bar{b}|S|\bar{a}\rangle = \delta_{ba} - 2\pi i \delta(E_b - E_a) \langle \bar{b}|\mathcal{T}|\bar{a}\rangle \quad (16.144)$$

where

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{CC'}{N!(N')!} \sum_P \delta_P \sum_{P'} \delta_{P'} \langle P'b|\mathcal{T}|Pa\rangle \quad (16.145)$$

and we have on the energy shell  $E = E_a = E_b$

$$\langle P'b|\mathcal{T}|Pa\rangle = \langle \Phi_{P'b}|V_P|\Psi_{P_a}^{(+)}\rangle \quad (16.146a)$$

and

$$\langle P'b|\mathcal{T}|Pa\rangle = \langle \Psi_{P'b}^{(-)}|V_P|\Phi_{P_a}\rangle \quad (16.146b)$$

or explicitly

$$\langle P'b|\mathcal{T}|Pa\rangle = \left\langle \Phi_{P'b} \left| V_P(\text{or } V_{P'}) + V_{P'} \frac{1}{E - H + i\varepsilon} V_P \right| \Phi_{P_a} \right\rangle. \quad (16.147)$$

We note that eq. (16.145) may also be written as

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{C'}{(N')!} \sum_{P'} \delta_{P'} \langle P'b|\mathcal{T}|\bar{a}\rangle \quad (16.148a)$$

or

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{C}{N!} \sum_P \delta_P \langle \bar{b}|\mathcal{T}|Pa\rangle. \quad (16.148b)$$

Finally, we may define the reduced  $T$ -matrix elements  $\bar{T}_{ba}$  on the momentum shell by the relation

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \delta(\mathbf{P}_b - \mathbf{P}_a) \bar{T}_{ba} \quad (16.149)$$

and the calculation of the cross sections proceeds as in Section 15.2, with  $T_{ba}$  replaced by  $\bar{T}_{ba}$ .

In view of future applications, it is worth looking in detail at some particular cases. First of all, if  $N = N'$ , so that the same number of identical "elementary" particles (of one kind) is present in the initial and final states (no creation or destruction of particles), we have

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{CC'}{[N!]^2} \sum_P \delta_P \sum_{P'} \delta_{P'} \langle P'b|\mathcal{T}|Pa\rangle.$$

From eqs. (16.148), we also have

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{C'}{N!} \sum_{P'} \delta_{P'} \langle P'b|\mathcal{T}|\bar{a}\rangle, \quad (16.150a)$$

or

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{C}{N!} \sum_P \delta_P \langle \bar{b}|\mathcal{T}|Pa\rangle. \quad (16.150b)$$

Using the fact that the states  $|\bar{a}\rangle$  and  $|\bar{b}\rangle$  are fully symmetrized, and dropping unnecessary prime symbols, we see that eqs. (16.150) reduce to

$$\langle \bar{b}|\mathcal{T}|\bar{a}\rangle = \frac{CC'}{N!} \sum_P \delta_P \langle Pb|\mathcal{T}|a\rangle \quad (16.151a)$$

and

$$\langle \bar{b} | \mathcal{T} | \bar{a} \rangle = \frac{CC'}{N!} \sum_P \delta_P \langle b | \mathcal{T} | Pa \rangle. \quad (16.151b)$$

As a further restriction, we now assume that there are  $N = N_0 + 1$  identical particles in the initial and final states, with  $N_0$  particles being bound in the target before and after the collision. We then have [see eq. (16.115)]

$$C = C' = \sqrt{N} = \sqrt{N_0 + 1} \quad (16.152)$$

and eqs. (16.151) become

$$\langle \bar{b} | \mathcal{T} | \bar{a} \rangle = \frac{1}{N_0!} \sum_P \delta_P \langle Pb | \mathcal{T} | a \rangle, \quad (16.153a)$$

$$\langle \bar{b} | \mathcal{T} | \bar{a} \rangle = \frac{1}{N_0!} \sum_P \delta_P \langle b | \mathcal{T} | Pa \rangle. \quad (16.153b)$$

Now the  $N_0!$  permutations of the variables  $(q_1, \dots, q_{N_0})$  have no effect on  $\Phi_a$  and  $\Phi_b$ , while the interchange  $P_{0j}$  of the coordinate  $q_0$  with one of the  $q_j$ 's ( $j = 1, 2, \dots, N_0$ ) is such that [see eq. (16.117)]

$$\begin{aligned} \delta_{P_{0j}} P_{0j} \Phi_a(q_0, \dots, q_{j-1}, q_j, q_{j+1}, \dots, q_{N_0}) \\ = \pm \Phi_a(q_j, \dots, q_{j-1}, q_0, q_{j+1}, \dots, q_{N_0}) \end{aligned} \quad (16.154a)$$

and

$$\begin{aligned} \delta_{P_{0j}} P_{0j} \Phi_b(q_0, \dots, q_{j-1}, q_j, q_{j+1}, \dots, q_{N_0}) \\ = \pm \Phi_b(q_j, \dots, q_{j-1}, q_0, q_{j+1}, \dots, q_{N_0}). \end{aligned} \quad (16.154b)$$

Hence we may write for example eq. (16.151a) as

$$\langle \bar{b} | \mathcal{T} | \bar{a} \rangle = \langle b | \mathcal{T} | a \rangle \pm \sum_{j=1}^{N_0} \langle P_{0j} b | \mathcal{T} | a \rangle \quad (16.155)$$

with the plus sign for bosons and the minus sign for fermions. Using the fact that

$$\langle P_{0j} b | \mathcal{T} | a \rangle = \langle P_{0k} b | \mathcal{T} | a \rangle, \quad (j, k = 1, 2, \dots, N_0) \quad (16.156)$$

we may also write

$$\langle \bar{b} | \mathcal{T} | \bar{a} \rangle = \langle b | \mathcal{T} | a \rangle \pm N_0 \langle P_{0j} b | \mathcal{T} | a \rangle \quad (16.157)$$

which is our final result. The matrix element  $\langle b | \mathcal{T} | a \rangle$  is often called the *direct* (unsymmetrized) transition matrix element. Explicitly, one has (on the energy shell) [26]

$$\langle b | \mathcal{T} | a \rangle = \left\langle \Phi_b \left| V_d + V_d \frac{1}{E - H + i\epsilon} V_d \right| \Phi_a \right\rangle \quad (16.158)$$



where  $V_d$  accounts for the total interaction between the particle "0" (with coordinates  $q_0$ ) and the remaining particles of the system [27]. The other quantity  $\langle P_{0j}b|\mathcal{T}|a\rangle$  appearing in eq. (16.157) is called an *exchange* transition matrix element. It is given explicitly by

$$\langle P_{0j}b|\mathcal{T}|a\rangle = \left\langle \Phi_{P_{0j}b} \left| V_d(\text{or } V_{P_{0j}}) + V_{P_{0j}} \frac{1}{E - H + i\varepsilon} V_d \right| \Phi_a \right\rangle \quad (16.159)$$

where  $V_{P_{0j}}$  is obtained from  $V_d$  by interchanging the roles of the particles "0" and "j". In terms of the reduced transition matrix elements on the momentum shell [see eq. (16.149)] we may write eq. (16.157) as

$$\bar{T}_{ba} = T_{ba}^d \pm N_0 T_{ba}^{\text{ex}} \quad (16.160)$$

where we have defined the objects  $T_{ba}^d$  and  $T_{ba}^{\text{ex}}$  by the relations

$$\langle b|\mathcal{T}|a\rangle = \delta(\mathbf{P}_b - \mathbf{P}_a) T_{ba}^d \quad (16.161)$$

and

$$\langle P_{0j}b|\mathcal{T}|a\rangle = \delta(\mathbf{P}_b - \mathbf{P}_a) T_{ba}^{\text{ex}}. \quad (16.162)$$

We shall illustrate the use of eq. (16.160) in Part IV of this book where we analyze various electron-atom and nucleon-nucleus collision processes. Of course, when the system contains only  $N = 2$  identical particles, eq. (16.160) leads directly to the results of Chapter 7.

## 16.7. Invariance principles and the collision matrix

This section is devoted to a brief account [28] of the role of invariance principles in collision processes. We first recall that in quantum theory invariance laws correspond to *symmetries* of the Schrödinger equation, i.e. to symmetries of the Hamiltonian operator of the system.

Consider for example a Hermitian operator  $A$  which commutes with the total Hamiltonian  $H$ , i.e.

$$[A, H] = 0 \quad (16.163)$$

and is therefore a *constant of the motion*. We shall also assume that  $A$  commutes with the channel Hamiltonians  $H_c$ . Then, from the definition (14.155) of the transition operator, we infer that

$$[A, \mathcal{T}_{fi}] = 0 \quad (16.164)$$

and also

$$[A, S_{fi}] = 0. \quad (16.165)$$

Hence, if  $\lambda'$  and  $\lambda''$  are two eigenvalues of the operator  $A$ , we have

$$\langle \lambda''|[A, \mathcal{T}_{fi}]|\lambda'\rangle = (\lambda'' - \lambda')\langle \lambda''|\mathcal{T}_{fi}|\lambda'\rangle = 0 \quad (16.166)$$

so that

$$\langle \lambda'' | \mathcal{T}_{fi} | \lambda' \rangle = \delta_{\lambda'' \lambda'} \mathcal{T}_{fi}(\lambda') \quad (16.167a)$$

or

$$\langle \lambda'' | \mathcal{T}_{fi} | \lambda' \rangle = \delta(\lambda'' - \lambda') \mathcal{T}_{fi}(\lambda'). \quad (16.167b)$$

We have already illustrated these equations in Section 14.4 when we were dealing with momentum and energy conservation. In the first case the operator  $A$  is given by  $\mathbf{P}$ , the total momentum operator of the system. The meaning of eq. (16.163) is then the following: to any infinitesimal spatial translation corresponding to a displacement  $\boldsymbol{\varepsilon}$  we may associate the unitary operator

$$T(\boldsymbol{\varepsilon}) = 1 - \frac{i}{\hbar}(\mathbf{P} \cdot \boldsymbol{\varepsilon}) \quad (16.168)$$

so that  $\mathbf{P}$  is the *generator* of infinitesimal translations. Moreover, the operator corresponding to a finite translation by an amount  $\mathbf{a}$  is given by

$$T(\mathbf{a}) = \exp\left(-\frac{i}{\hbar}\mathbf{P} \cdot \mathbf{a}\right). \quad (16.169)$$

Let us require that the Hamiltonian be invariant with respect to translations, namely

$$H = THT^\dagger$$

or

$$HT = TH \quad (16.170)$$

i.e.

$$[T, H] = 0. \quad (16.171)$$

Since a necessary and sufficient condition for  $H$  to be invariant under translations is that it must be invariant with respect to infinitesimal translations, we see from eqs. (16.168) and (16.171) that the condition (16.163), namely

$$[\mathbf{P}, H] = 0 \quad (16.172)$$

expresses the invariance of  $H$  with respect to *spatial translations*.

In the case of energy conservation, the operator is the Hamiltonian  $H$  itself, which is the generator of infinitesimal *time translations* [see eq. (13.14)].

Let us now consider *rotations*. In this case the operator corresponding to an infinitesimal rotation of angle  $\varepsilon$  in the positive (right-handed) sense about an oriented axis defined by the unit vector  $\hat{\mathbf{u}}$  is given by

$$R_{\mathbf{u}}(\varepsilon) = 1 - \frac{i\varepsilon}{\hbar}(\mathbf{J} \cdot \hat{\mathbf{u}}) \quad (16.173)$$

where the generator  $\mathbf{J}$  is the total angular momentum operator of the system. Invariance with respect to rotations is thus expressed by

$$[\mathbf{J}, H] = 0 \quad (16.174)$$

which leads to the conservation of angular momentum. Since  $\mathbf{J}$  also commutes with  $H_c$  we see that

$$[\mathbf{J}, S_{fi}] = 0 \quad (16.175)$$

and

$$[\mathbf{J}, \mathcal{T}_{fi}] = 0. \quad (16.176)$$

However, since the operators  $\mathbf{P}$  and  $\mathbf{J}$  do not in general commute, eq. (14.174) cannot be further reduced in terms of – for example – the eigenstates of  $J^2$  and  $J_z$ . Only in the *center of mass system* where the eigenvalue of  $\mathbf{P}$  vanishes and therefore  $[\mathbf{P}, \mathbf{J}] = 0$ , are we allowed to diagonalize simultaneously the operators  $\mathbf{P}$ ,  $J^2$  and  $J_z$ .

Assuming that we are working in the center of mass system, let us look more closely at the consequences of eqs. (16.167) and (16.176). Let us denote by  $|\bar{a}\rangle$  a correctly symmetrized initial state (see Section 16.6) which we develop in eigenstates of the operators  $J^2$  and  $J_z$  as

$$|\bar{a}\rangle = \sum_{j_a} \sum_{m_a} C_{j_a, m_a} |\bar{a}, j_a, m_a\rangle \quad (16.177)$$

where  $C_{j_a, m_a}$  are numerical factors, while

$$J^2 |\bar{a}, j_a, m_a\rangle = j_a(j_a + 1) \hbar^2 |\bar{a}, j_a, m_a\rangle \quad (16.178)$$

and

$$J_z |\bar{a}, j_a, m_a\rangle = m_a \hbar |\bar{a}, j_a, m_a\rangle. \quad (16.179)$$

Similarly, we write

$$|\bar{b}\rangle = \sum_{j_b} \sum_{m_b} C_{j_b, m_b} |\bar{b}, j_b, m_b\rangle \quad (16.180)$$

with

$$J^2 |\bar{b}, j_b, m_b\rangle = j_b(j_b + 1) \hbar^2 |\bar{b}, j_b, m_b\rangle \quad (16.181)$$

and

$$J_z |\bar{b}, j_b, m_b\rangle = m_b \hbar |\bar{b}, j_b, m_b\rangle. \quad (16.182)$$

Then, using eqs. (16.167), we have

$$\langle \bar{b}, j_b, m_b | \mathcal{T} | \bar{a}, j_a, m_a \rangle = \delta(\mathbf{P}_b - \mathbf{0}) \delta_{j_b, j_a} \delta_{m_b, m_a} T_{\bar{b}\bar{a}}^-(\mathbf{P}_a = \mathbf{0}, j_a, m_a) \quad (16.183)$$

where  $T_{\bar{b}\bar{a}}^-$  is now a “super-reduced” transition matrix element. Moreover, a simple calculation using eq. (16.176) shows that the object  $T_{\bar{b}\bar{a}}^-$  is independent of  $m_a$ . Thus we may write

$$\langle \bar{b}, j_b, m_b | \mathcal{T} | \bar{a}, j_a, m_a \rangle = \delta(\mathbf{P}_b - \mathbf{0}) \delta_{j_b, j_a} \delta_{m_b, m_a} T_{\bar{b}\bar{a}}^-(\mathbf{P}_a = \mathbf{0}, j_a) \quad (16.184)$$

so that the transition matrix element is *diagonal in  $j$  and  $m$  and independent of  $m$* .

Another important symmetry operation which leaves the Hamiltonian invariant is the *permutation  $P$  of identical particles*. In any such permutation

$$[P, H] = 0. \quad (16.185)$$

Furthermore, according to the symmetrization postulate the projectors  $\mathcal{P}_s$  and  $\mathcal{P}_A$  into the symmetrical and antisymmetrical states are also constants of the motion.

We now consider the *reflection invariance*, leading to the *conservation of parity*. The parity operator  $\mathcal{P}$  is a linear, unitary operator such that the polar vectors  $\mathbf{r}$  (coordinates) and  $\mathbf{p}$  (momenta) change sign, while the axial vectors  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$  (orbital angular momentum) and  $s$  (spin) are invariant. Thus

$$\begin{aligned}\mathcal{P}\mathbf{r}\mathcal{P}^\dagger &= -\mathbf{r}, & \mathcal{P}\mathbf{p}\mathcal{P}^\dagger &= -\mathbf{p}, \\ \mathcal{P}\mathbf{L}\mathcal{P}^\dagger &= \mathbf{L}, & \mathcal{P}s\mathcal{P}^\dagger &= s.\end{aligned}\quad (16.186)$$

These equations define the operator  $\mathcal{P}$  up to a phase. In addition

$$\mathcal{P}^2 = I \quad (\text{or } \mathcal{P} = \mathcal{P}^\dagger) \quad (16.187)$$

so that the phase of  $\mathcal{P}$  is now determined to within a sign and the eigenvalues of  $\mathcal{P}$  are  $\pm 1$ . To determine completely the operator  $\mathcal{P}$ , we may specify how it acts on the basis vectors of a given representation. For example, if we choose the position representation  $\{\mathbf{r}\}$  and denote by  $\alpha$  the remaining quantum numbers, we may define (for one particle)

$$\mathcal{P}\psi(\mathbf{r}, \alpha) = \psi(-\mathbf{r}, \alpha) \quad (16.188)$$

and for several particles

$$\mathcal{P}\psi(\mathbf{r}_1, \mathbf{r}_2, \dots; \alpha_1, \alpha_2, \dots) = \psi(-\mathbf{r}_1, -\mathbf{r}_2, \dots; \alpha_1, \alpha_2, \dots). \quad (16.189)$$

With this choice we see that the eigenvalue  $+1$  of  $\mathcal{P}$  corresponds to wave functions of *positive parity*, i.e. such that

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots; \alpha_1, \alpha_2, \dots) = \psi(-\mathbf{r}_1, -\mathbf{r}_2, \dots; \alpha_1, \alpha_2, \dots) \quad (16.190)$$

while the eigenvalue  $-1$  corresponds to wave functions having *negative parity*, namely

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots; \alpha_1, \alpha_2, \dots) = -\psi(-\mathbf{r}_1, -\mathbf{r}_2, \dots; \alpha_1, \alpha_2, \dots). \quad (16.191)$$

For all but the weak interactions it is believed that parity is conserved, so that

$$[\mathcal{P}, H] \doteq [\mathcal{P}, H_c] = 0. \quad (16.192)$$

Thus we also have

$$[\mathcal{P}, S_{fi}] = 0 \quad (16.193)$$

and

$$[\mathcal{P}, \mathcal{T}_{fi}] = 0. \quad (16.194)$$

It is also worth noting that from eqs. (16.186)

$$\mathcal{P}\mathbf{J}\mathcal{P}^\dagger = \mathbf{J}. \quad (16.195)$$

Hence the parity operator commutes with the total angular momentum  $\mathbf{J}$  and the reflection operation commutes with the rotations.

It is sometimes convenient to relax somewhat the phase convention adopted in the definition of  $\mathcal{P}$ . For example, instead of eq. (16.188) we may require that

$$\mathcal{P}\psi(\mathbf{r}, \alpha) = \zeta\psi(-\mathbf{r}, \alpha) \quad (16.196)$$

where  $\zeta = \pm 1$  is called the *intrinsic parity* of the particle. More generally, for a system of  $N$  particles

$$\begin{aligned} \mathcal{P}\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N; \alpha_1, \alpha_2, \dots, \alpha_N) \\ = \zeta_1 \zeta_2 \dots \zeta_N \psi(-\mathbf{r}_1, -\mathbf{r}_2, \dots, -\mathbf{r}_N; \alpha_1, \alpha_2, \dots, \alpha_N) \end{aligned} \quad (16.197)$$

where the factors  $\zeta_1, \zeta_2, \dots, \zeta_N$  are so chosen that  $\mathcal{P}$  commutes [29] with  $H$ . The concept of intrinsic parity is only useful when the number of particles can change. Otherwise, as in elementary quantum theory, one may simply take  $\zeta = +1$  for every particle.

We conclude this section by a discussion of *time-reversal invariance*. We first note that, as for spatial translations, time translations and rotations, this type of invariance also occurs in Classical Mechanics [30]. Indeed, let us start from Newton's law of motion for a mass point, namely

$$m \frac{d^2 \mathbf{r}}{dt^2} = \mathbf{F} \quad (16.198)$$

and assume that the force  $\mathbf{F}$  only depends explicitly on the position coordinates. Then, because Newton's equations are of second order in  $t$ , we can associate to every solution  $\mathbf{r}(t)$  of eq. (16.198) another solution

$$\mathbf{r}'(t) = \mathbf{r}(-t). \quad (16.199)$$

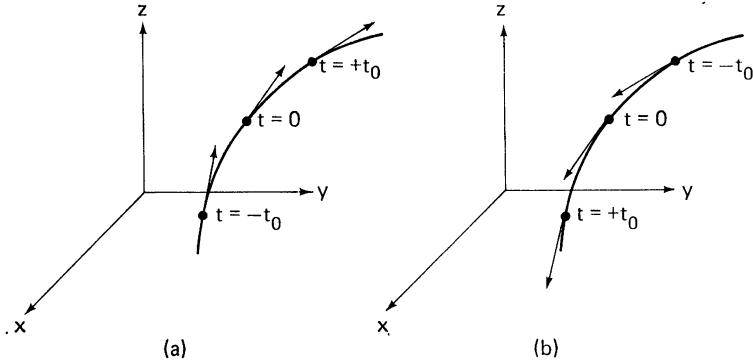


Fig. 16.1. Two classical trajectories (a) and (b) which correspond by time reversal.

The correspondence between the two solutions is illustrated on Fig. 16.1. We note that the position of the particle at time  $t_0$  in case (a) is the same as its position at time  $-t_0$  in case (b), while the velocities and momenta are reversed. Indeed,

$$\mathbf{v}'(t_0) = \left[ \frac{d\mathbf{r}'(t)}{dt} \right]_{t_0} = - \left[ \frac{d\mathbf{r}(-t)}{d(-t)} \right]_{t_0} = - \left[ \frac{d\mathbf{r}(t')}{dt'} \right]_{-t_0} = -\mathbf{v}(-t_0). \quad (16.200)$$

Let us now investigate the question of time reversal in quantum theory. We begin by considering the case of a spinless particle moving in a real potential  $V(\mathbf{r})$ . We write the Schrödinger equation as

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}, t). \quad (16.201)$$

We now change  $t$  into  $-t$ . Since the Hamiltonian is real, we may restore the form of eq. (16.201) by taking the complex conjugate. Thus

$$i\hbar \frac{\partial}{\partial t} \Psi^*(\mathbf{r}, -t) = \left[ -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \right] \Psi^*(\mathbf{r}, -t). \quad (16.202)$$

Hence, if  $\Psi(\mathbf{r}, t)$  is a solution of the Schrödinger equation, so is also the wave function

$$\Psi'(\mathbf{r}, t) = \Psi^*(\mathbf{r}, -t). \quad (16.203)$$

We note that this result depends on our choice of representation. For example, if we write

$$\Psi(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int \phi(\mathbf{p}, t) \exp\left\{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}\right\} d\mathbf{p}$$

and

$$\Psi'(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int \phi'(\mathbf{p}, t) \exp\left\{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}\right\} d\mathbf{p}$$

then eq. (16.203) implies that

$$\phi'(\mathbf{p}, t) = \phi^*(-\mathbf{p}, -t) \quad (16.204)$$

and we see that in momentum space we have to change  $\mathbf{p}$  into  $-\mathbf{p}$  as we transform  $t$  into  $-t$ . This precisely agrees with the result obtained in Classical Mechanics.

We may summarize the results obtained until now in the following way. Suppose that we define a transformation of the observables which leaves  $\mathbf{r}$  unchanged but carries  $\mathbf{p}$  into  $-\mathbf{p}$ . We denote the corresponding operator by  $\mathcal{K}$  and call it the *time reversal operator*. Thus

$$\mathcal{K} \mathbf{r} \mathcal{K}^\dagger = \mathbf{r}$$

and

$$\mathcal{K} \mathbf{p} \mathcal{K}^\dagger = -\mathbf{p}. \quad (16.205)$$

It is not difficult to find the operator  $\mathcal{K}$  in the simple case which we have discussed so far. Indeed, if we denote by  $K_0$  the *complex conjugate operator* corresponding to the *position* representation, we may take

$$\mathcal{K} = K_0 \quad (16.206)$$

since in the position representation  $\mathbf{r}$  is purely real and  $\mathbf{p} = -i\hbar \nabla_{\mathbf{r}}$  purely imaginary. Because the Hamiltonian appearing in eq. (16.201) is invariant when  $\mathbf{p}$  is changed into  $-\mathbf{p}$ , we see that

$$[\mathcal{K}, H] = 0. \quad (16.207)$$

We may then rewrite eq. (16.203) as

$$\Psi'(\mathbf{r}, t) = \mathcal{K}\Psi(\mathbf{r}, -t). \quad (16.208)$$

We note that the operator  $K_0$  is anti-unitary [31] and such that  $K_0^2 = I$  or  $K_0 = K_0^\dagger$ . The occurrence of anti-unitary operators should come as no surprise since in quantum theory two systems are equivalent if they are connected by a unitary or an anti-unitary transformation [32]. Furthermore, the operator  $\mathcal{K}$  as defined by eqs. (16.205) anticommutes with the components of the orbital angular momentum  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ , i.e.

$$\mathcal{K}\mathbf{L}\mathcal{K}^\dagger = -\mathbf{L}. \quad (16.209)$$

This last property suggests a natural extension of the time reversal operator when it is acting on the spin variables: we then require that the spin should change sign under the  $\mathcal{K}$  transformation, namely

$$\mathcal{K}\mathbf{s}\mathcal{K}^\dagger = -\mathbf{s}. \quad (16.210)$$

Consequently  $\mathcal{K}$  also anticommutes with the total angular momentum

$$\mathcal{K}\mathbf{J}\mathcal{K}^\dagger = -\mathbf{J}. \quad (16.211)$$

For a spin one-half particle a simple calculation shows that the operator  $\mathcal{K}$  may be written as

$$\mathcal{K} = \tau K_0 \quad (16.212)$$

with  $\tau = i\sigma_y$ . Here  $\sigma_y$  is the second of the Pauli spin matrices [33].

We now consider the general case, starting from the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = H\Psi(t) \quad (16.213)$$

where we assume the total Hamiltonian  $H$  to be time-independent. We first change  $t$  into  $-t$  and then apply the operator  $K_0$  of complex conjugation. This yields [34]

$$i\hbar \frac{\partial}{\partial t} \Psi^*(-t) = H^*\Psi^*(-t). \quad (16.214)$$

We have already seen that if  $H = H^*$  then  $\Psi'(t) = K_0\Psi(-t)$  is also a solution of the Schrödinger equation, describing the *time-reversed state* of the system associated with  $\Psi(t)$ . In general, however,  $H^* \neq H$ . In this case we suppose that there exists a unitary operator  $\tau$  such that [35]

$$\tau H^* \tau^\dagger = H. \quad (16.215)$$

Obviously, the operator  $\tau$  should not contain  $K_0$  and should become the identity when  $H$  is real. Operating on the left on both sides of eq. (16.214) with  $\tau$  and using eq. (16.215), we find that

$$i\hbar \frac{\partial}{\partial t} \tau \Psi^*(-t) = H\tau \Psi^*(-t). \quad (16.216)$$

Thus, if  $\Psi(t)$  is a solution of the Schrödinger equation, so is also

$$\Psi'(t) = \tau \Psi^*(-t) \quad (16.217)$$

or

$$\Psi'(t) = \mathcal{K} \Psi(-t) \quad (16.218)$$

where

$$\mathcal{K} = \tau K_0. \quad (16.219)$$

In analogy with our above discussion we call  $\Psi'(t)$  the time-reversed state vector associated with  $\Psi(t)$ . We note that since  $K_0$  is anti-unitary and  $\tau$  is unitary the operator  $\mathcal{K}$  defined by eq. (16.219) is anti-unitary.

Let us return once more to the Schrödinger equation (16.213). Reversing the time and inserting  $\mathcal{K}^\dagger \mathcal{K} (= I)$  between  $H$  and  $\Psi$ , we get

$$-i\hbar \frac{\partial}{\partial t} \Psi(-t) = H \mathcal{K}^\dagger \mathcal{K} \Psi(-t) \quad (16.220)$$

or

$$-\mathcal{K} i\hbar \frac{\partial}{\partial t} \Psi(-t) = \mathcal{K} H \mathcal{K}^\dagger \mathcal{K} \Psi(-t).$$

Now, using eqs. (16.217)–(16.219), we find that

$$-\tau K_0 i\hbar \frac{\partial}{\partial t} \Psi(-t) = -\tau(-i)\hbar \frac{\partial}{\partial t} \Psi^*(-t) = \mathcal{K} H \mathcal{K}^\dagger \Psi'(t)$$

or

$$i\hbar \frac{\partial}{\partial t} \Psi'(t) = \mathcal{K} \mathcal{K}^\dagger \Psi'(t) \quad (16.221)$$

which we want to be identical with

$$i\hbar \frac{\partial}{\partial t} \Psi'(t) = H \Psi'(t). \quad (16.222)$$

Therefore, provided the operator  $\tau$  satisfying eq. (16.215) exists, we see that the requirement

$$\mathcal{K} H \mathcal{K}^\dagger = H \quad (16.223)$$

or

$$[\mathcal{K}, H] = 0 \quad (16.224)$$

is the necessary and sufficient condition for the time-reversal invariance of the system governed by the time-independent Hamiltonian  $H$ .

We now return more specifically to collision problems. We assume that the operators  $H$ ,  $H_c$  and  $V_c$  are invariant under time reversal. That is

$$\mathcal{K} H \mathcal{K}^\dagger = H, \quad \mathcal{K} H_c \mathcal{K}^\dagger = H_c, \quad \mathcal{K} V_c \mathcal{K}^\dagger = V_c \quad (16.225)$$

for all channels  $c$ .



Let us first consider the channel Hamiltonian  $H_c$ , such that

$$H_c \Phi_n = E_n \Phi_n, \quad n \equiv (c, \gamma) \quad (16.226)$$

and let  $A_i (i = 1, 2, \dots)$  be a complete set of observables, including  $H_c$ , which specify the channel eigenfunctions  $\Phi_n$ . For example, the  $A_i$  may correspond to the angular momentum, spin, isospin, parity, etc. of the states  $\Phi_n$ . We have

$$A_i \Phi_n = a_i \Phi_n. \quad (16.227)$$

Now, most observables lead to operators which are either even or odd under the time-reversal operator  $\mathcal{K}$ . That is

$$A'_i = \mathcal{K} A_i \mathcal{K}^\dagger = \pm A_i \quad (16.228)$$

so that

$$A_i \Phi'_n = \pm a_i \Phi'_n \quad (16.229)$$

with

$$\Phi'_n = \mathcal{K} \Phi_n. \quad (16.230)$$

Therefore, if we choose the observables satisfying eq. (16.228) to classify the states, we see that  $\Phi_n$  and  $\Phi'_n$  belong to the same set. If we denote by  $(-n)$  the time-reversed state of  $n$ , i.e. the state obtained from  $n$  by reversing the sign of all linear momenta, angular momenta and spins of the system, we see that

$$\Phi'_n = \mathcal{K} \Phi_n = \mu_{-n} \Phi_{-n} \quad (16.231)$$

where  $\Phi_{-n}$  is one of the states  $\Phi_n$  and  $\mu_{-n}$  is a phase factor such that  $|\mu_{-n}| = 1$ . For example, if

$$\Phi_n = (2\pi)^{-3/2} \exp(ik \cdot r) \quad (16.232)$$

then

$$\Phi'_n = \Phi_{-n} = (2\pi)^{-3/2} \exp(-ik \cdot r) = \Phi_n^*. \quad (16.233)$$

Let us now look at the state vector

$$\Psi_n^{(\pm)} = \Phi_n + \frac{1}{E_n - H \pm i\varepsilon} V_c \Phi_n. \quad (16.234)$$

Applying the time-reversal operator  $\mathcal{K}$  and taking into account eq. (16.231), we find that

$$\begin{aligned} \mathcal{K} \Psi_n^{(\pm)} &= \mathcal{K} \left( 1 + \frac{1}{E_n - H \pm i\varepsilon} V_c \right) \mathcal{K}^\dagger \mathcal{K} \Phi_n \\ &= \mu_{-n} \left[ \left( 1 + \frac{1}{E_n - H \mp i\varepsilon} V_c \right) \Phi_{-n} \right] = \mu_{-n} \Psi_{-n}^{(\mp)}. \end{aligned} \quad (16.235)$$

Hence, from eqs. (16.231) and (16.235) we see that

$$\begin{aligned} \mathcal{K} \Phi_a &= \mu_{-a} \Phi_{-a}, \\ \mathcal{K} \Phi_b &= \mu_{-b} \Phi_{-b}, \\ \mathcal{K} \Psi_a^{(\pm)} &= \mu_{-a} \Psi_{-a}^{(\mp)} \end{aligned} \quad (16.236)$$

and

$$\mathcal{K} \Psi_b^{(\pm)} = \mu_{-b} \Psi_{-b}^{(\mp)}$$

so that the transition matrix element  $\langle b|\mathcal{T}|a\rangle$  corresponding to a collision process  $a \rightarrow b$  is such that

$$\begin{aligned}
 \langle b|\mathcal{T}|a\rangle &= \left\langle \Phi_b \left| V_i + V_f \frac{1}{E_a - H + i\varepsilon} V_i \right| \Phi_a \right\rangle \\
 &= \left( \mathcal{K} \left[ V_i + V_f \frac{1}{E_a - H + i\varepsilon} V_i \Phi_a \right], \mathcal{K} \Phi_b \right) \\
 &= \mu_{-a}^* \mu_{-b} \left( \left[ V_i + V_f \frac{1}{E_a - H - i\varepsilon} V_i \right] \Phi_{-a}, \Phi_{-b} \right) \\
 &= \mu_{-a}^* \mu_{-b} \left\langle \Phi_{-a} \left| V_i + V_i \frac{1}{E_a - H + i\varepsilon} V_f \right| \Phi_{-b} \right\rangle, \quad (16.237)
 \end{aligned}$$

where we have used the notation  $(\mathbf{a}, \mathbf{b})$  to denote the scalar product of the two vectors  $\mathbf{a}$  and  $\mathbf{b}$ . Now, on the energy shell, we have

$$\langle \Phi_{-a} | V_i | \Phi_{-b} \rangle = \langle \Phi_{-a} | V_f | \Phi_{-b} \rangle$$

so that eq. (16.237) becomes

$$\langle b|\mathcal{T}|a\rangle = \mu_{-a}^* \mu_{-b} \langle (-a)|\mathcal{T}|(-b)\rangle. \quad (16.238)$$

More explicitly, in terms of channel indices, we have

$$\langle f, \beta | \mathcal{T} | i, \alpha \rangle = \mu_{i, -\alpha}^* \mu_{f, -\beta} \langle i, (-\alpha) | \mathcal{T} | f, (-\beta) \rangle \quad (16.239)$$

which is known as the *reciprocity theorem* or *microreversibility relation*. Thus, up to a phase factor, the transition matrix element between an initial state and a final state having the same energy is equal to the transition matrix element between the final and the initial state with all eigenvalues of odd operators under time reversal describing these states reversed in sign. It is believed that the reciprocity theorem (16.239) is one of the fundamental symmetry relations which are satisfied by physical systems.

As an application of these considerations, we consider the reaction



in the center of mass system. Let us denote by  $S_A, S_B, S_C, S_D$  the spins of the particles involved in the reaction (16.240), and by  $\mathbf{k}_i$  and  $\mathbf{k}_f$  the relative wave vectors in the initial and final states. Then, from the reciprocity theorem (16.239), we obtain for the reduced  $T$ -matrix element

$$\langle \mathbf{k}_f, S_C, S_D | T | \mathbf{k}_i, S_A, S_B \rangle = \langle -\mathbf{k}_i, -S_A, -S_B | T | -\mathbf{k}_f, -S_C, -S_D \rangle. \quad (16.241)$$

Summing over initial and final spin states, we have

$$\begin{aligned}
 \sum_{\text{spin}} |\langle \mathbf{k}_f, S_C, S_D | T | \mathbf{k}_i, S_A, S_B \rangle|^2 \\
 = \sum_{\text{spin}} |\langle -\mathbf{k}_i, -S_A, -S_B | T | -\mathbf{k}_f, -S_C, -S_D \rangle|^2. \quad (16.242)
 \end{aligned}$$

To be invariant with respect to rotations, this expression must only be a function of the scalar products  $k_i^2$ ,  $k_f^2$ , and  $\mathbf{k}_i \cdot \mathbf{k}_f$ . We may thus rewrite the right-hand side of eq. (16.242) as

$$\sum_{\text{spin}} |\langle -\mathbf{k}_i, -S_A, -S_B | T | -\mathbf{k}_f, -S_C, -S_D \rangle|^2 = \sum_{\text{spin}} |\langle \mathbf{k}_i, S_A, S_B | T | \mathbf{k}_f, S_C, S_D \rangle|^2 \quad (16.243)$$

where we have also used the fact that the spins are dummy indices in the sum. Hence, from eqs. (16.242) and (16.243) we deduce that

$$\sum_{\text{spin}} |\langle \mathbf{k}_f, S_C, S_D | T | \mathbf{k}_i, S_A, S_B \rangle|^2 = \sum_{\text{spin}} |\langle \mathbf{k}_i, S_A, S_B | T | \mathbf{k}_f, S_C, S_D \rangle|^2 \quad (16.244)$$

so that in the evaluation of cross sections the *dynamical part*, i.e. the square of the modulus of the  $T$ -matrix element, is the same for the direct reaction (16.240) and for the inverse reaction

$$C + D \rightarrow A + B. \quad (16.245)$$

The only difference in evaluating cross sections appears in the *kinematical* factors involved in the density of final states. From eqs. (15.27), (15.41) and (15.51) we deduce that for *unpolarized beams* the differential cross section for the *direct* reaction (16.240) is given by

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{DIR}} = \alpha \frac{k_f}{k_i} \frac{1}{(2S_A + 1)(2S_B + 1)} \sum_{\text{spin}} |\langle \mathbf{k}_f, S_C, S_D | T | \mathbf{k}_i, S_A, S_B \rangle|^2, \quad (16.246)$$

with

$$\alpha = \frac{(2\pi)^4}{\hbar^4 c^4 (1/E_A + 1/E_B)(1/E_C + 1/E_D)}.$$

For the *inverse reaction* (16.245), we have instead

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{INV}} = \alpha \frac{k_i}{k_f} \frac{1}{(2S_C + 1)(2S_D + 1)} \sum_{\text{spin}} |\langle \mathbf{k}_i, S_A, S_B | T | \mathbf{k}_f, S_C, S_D \rangle|^2. \quad (16.247)$$

Using eq. (16.244), we may also write eq. (16.247) as

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{INV}} = \alpha \frac{k_i}{k_f} \frac{1}{(2S_C + 1)(2S_D + 1)} \sum_{\text{spin}} |\langle \mathbf{k}_f, S_C, S_D | T | \mathbf{k}_i, S_A, S_B \rangle|^2. \quad (16.248)$$

Hence, by comparing eqs. (16.246) and (16.248), we conclude that for unpolarized beams

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{DIR}} (2S_A + 1)(2S_B + 1)k_i^2 = \left( \frac{d\sigma}{d\Omega} \right)_{\text{INV}} (2S_C + 1)(2S_D + 1)k_f^2. \quad (16.249)$$

This relation is usually known as the *principle of detailed balance*. It has many applications in atomic, nuclear [36] and elementary particle [37] collisions.

## References and notes

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- [5] We shall demonstrate in Section 18.1 that  $T_l(k)$  is related to the phase shift  $\delta_l$  by  $T_l(k) = -(\pi km)^{-1} \exp\{i\delta_l(k)\} \sin \delta_l(k)$ .
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- [14] We emphasize that the bound states  $\Psi^{(B)}$  are such that *all* the particles are bound. Partially bound states where some of the particles are bound together, are included in the continuum part of  $H$ .
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- [23] When there is more than one arrangement channel difficulties concerning the limiting process  $\epsilon \rightarrow 0^+$  and the uniqueness of the solution appear as in the discussion of the Lippmann-Schwinger equations.
- [24] We follow here the treatment of GOLDBERGER, M. L. and K. M. WATSON (1964), *Collision Theory* (Wiley, New York) Chapter 4, where an extensive discussion of the scattering of identical particles may be found.
- [25] We use here the symbol  $P$  to denote a permutation, as in Chapter 7.
- [26] We recall that we are considering here the matrix element  $\langle b|\mathcal{T}|a\rangle$  for a transition occurring in a system of  $N = N_0 + 1$  identical “elementary” particles. In general, of course, the on-the-energy shell transition matrix element  $\langle b|\mathcal{T}|a\rangle$  is given by eqs. (14.160), namely  $\langle b|\mathcal{T}|a\rangle = \langle \Phi_b|V_i(\text{or } V_f) + V_f(E - H + i\epsilon)^{-1} V_i|\Phi_a\rangle$ .
- [27] By “remaining particles of the system” we mean the  $N_0$  other “identical” particles, together with one or several different particles. For example, in electron-atom scattering

the potential  $V_d$  contains the interactions between the electron "0" and the  $N_0$  electrons of the target, plus the interaction between the electron "0" and the atomic nucleus.

- [28] For a detailed treatment of invariance principles in quantum theory we mention the following useful references:

WIGNER, E. P. (1959), *Group Theory* (Academic Press, New York);

MESSIAH, A. (1966), *Quantum Mechanics* (Wiley, New York) Vol. II, Chapter 15;

HAMERMESH, M. (1962), *Group Theory* (Addison-Wesley, Reading, Mass.);

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GOLDBERGER, M. L. and K. M. WATSON (1964), loc. cit. [24], Chapter 2.

- [29] If one cannot find an appropriate set of intrinsic parities such that  $[\mathcal{P}, H] = 0$ , the parity conservation law is violated; this is the case for weak interactions.

- [30] On the contrary the concept of parity does not appear in classical theory. This is easily understood in terms of the two first equations (16.186), which imply that  $\mathcal{P}\mathbf{r} = -\mathbf{r}\mathcal{P}$  and  $\mathcal{P}\mathbf{p} = -\mathbf{p}\mathcal{P}$ .

- [31] An *anti-unitary* operator  $\mathcal{K}$  is *antilinear*, i.e.  $\mathcal{K}(\alpha|a\rangle + \beta|b\rangle) = \alpha^*\mathcal{K}|a\rangle + \beta^*\mathcal{K}|b\rangle$  ( $\alpha$  and  $\beta$  complex constants) and also satisfies the relation  $\mathcal{K}\mathcal{K}^\dagger = \mathcal{K}^\dagger\mathcal{K} = I$ . We note that antilinear operators are such that  ${}_a\mathcal{K} = \mathcal{K}{}_a^*$ . Furthermore  $(\langle b|\mathcal{K})|a\rangle = [\langle b|(\mathcal{K}|a\rangle)]^*$ . Given an anti-unitary transformation of vectors and operators such that  $|a'\rangle = \mathcal{K}|a\rangle$ ,  $\langle b'| = \langle b|\mathcal{K}^\dagger$  and  $A' = \mathcal{K}A\mathcal{K}^\dagger$ , where  $A$  is a linear operator, one has  $\langle b'|A'|a'\rangle = \langle b|A|a\rangle^*$ . After this anti-unitary transformation, the relations between vectors and operators are maintained if we replace all coefficients by their complex conjugate. For example, the basic commutation relation  $[x, p_x] = i\hbar$  now becomes  $[x', p'_x] = -i\hbar$ .

- [32] The proof of this property follows from the following theorem: "If there exists a one-to-one correspondence  $\mathcal{R}$  of a linear space into itself, such that  $|\langle a|b\rangle| = |\langle a'|b'\rangle|$  with  $|a'\rangle = \mathcal{R}|a\rangle$ ,  $|b'\rangle = \mathcal{R}|b\rangle$  for any pair of vectors, then the phases may always be chosen so that  $\mathcal{R}$  is either unitary or antiunitary". Except for time reversal all the transformations considered in this section are unitary.

- [33] We recall that the Pauli spin matrices are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- [34] In eq. (16.214) we should understand  $\Psi^*$  as follows. Let  $\{c_i\}$  be the components of the state vector  $\Psi$  in a given representation. Then  $\Psi^*$  is the state vector having components  $\{c_i^*\}$  in the same basis system.

- [35] The unitarity condition on the operator  $\tau$  is imposed by the requirement of preserving the normalization [see eq. (16.217)].

- [36] See for example BLATT, J. M. and V. WEISSKOPF (1952), *Theoretical Nuclear Physics* (Wiley, New York) Chapters 10 and 12.

- [37] A particularly interesting application of this principle to elementary particle physics is the determination of the spin of the charged pion. See for example KÄLLEN, G. (1964), *Elementary Particle Physics* (Addison-Wesley, Reading, Mass.) Chapter 3.

## Two-Potential Scattering

Before we proceed to the last part of this book, devoted to some applications of collision theory, we shall consider in this chapter a class of problems which may be considerably simplified by using formal scattering theory. These are the so-called “two-potential” problems, such that the interaction may be broken in a physically meaningful way in two parts: one which is treated exactly, and the other which is handled in an approximate way. A natural framework to discuss these problems is the Furry picture which we introduce in Section 17.1. In the next section we obtain the generalized Lippmann–Schwinger equations, while the Gell-Mann and Goldberger [1] “two-potential” formulae are derived in Section 17.3. Finally, in Section 17.4 we discuss the distorted wave Born series. The theory of *final state interactions* which constitutes an important application of two-potential scattering will be discussed in Chapter 21.

### 17.1. The Furry picture

We consider a collision such that in the initial arrangement channel

$$H = H_i + V_i \quad (17.1a)$$

while in the final arrangement channel

$$H = H_f + V_f. \quad (17.1b)$$

Let us assume that the interaction potentials  $V_i$  and  $V_f$  may be split as

$$V_i = U_i + W_i \quad (17.2a)$$

and

$$V_f = U_f + W_f. \quad (17.2b)$$

A typical example is the scattering of particles under the combined influence of the Coulomb and nuclear interactions, which we already considered in Section 6.3. In what follows, however, we shall derive general formulae without making any particular choice concerning the nature of the potentials appearing in eqs. (17.2).

Let us consider the new Hamiltonians

$$\bar{H}_i = H_i + U_i \quad (17.3a)$$

and

$$\bar{H}_f = H_f + U_f \quad (17.3b)$$

which already contain the interactions  $U_i$  and  $U_f$ . We suppose that  $\bar{H}_i$  and  $\bar{H}_f$  correspond to scattering problems *which are already solved*. More generally, we write for a given arrangement channel  $c$  that

$$H = H_c + V_c, \quad H_c \Phi_n = E_n \Phi_n, \quad V_c = U_c + W_c, \quad \bar{H}_c = H_c + U_c \quad (17.4)$$

and we recall that the “free” waves  $\Phi_n$  describe the system when the “particles” (elementary or complex) belonging to the arrangement channel  $c$  do not interact.

Let us suppose that we are able to solve the Lippmann–Schwinger equations

$$\chi_n^{(\pm)} = \Phi_n + \frac{1}{E_n - H_c \pm i\varepsilon} U_c \chi_n^{(\pm)} \quad (17.5)$$

which determine the *distorted waves*  $\chi_n^{(\pm)}$ . We may also write

$$\chi_n^{(\pm)} = \Phi_n + \frac{1}{E_n - \bar{H}_c \pm i\varepsilon} U_c \Phi_n \quad (17.6)$$

where we have introduced the new Green’s operators

$$\bar{G}_c^{(\pm)} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_n - \bar{H}_c \pm i\varepsilon}. \quad (17.7)$$

The distorted waves  $\chi_n^{(\pm)}$  clearly correspond to the free waves  $\Phi_n$ , distorted by the presence of the interaction  $U_c$ . In what follows we shall take advantage of our knowledge of the distorted waves in order to obtain useful expressions for the transition matrix element. The fact that the total Hamiltonian may be written as

$$H = \bar{H}_c + W_c = H_c + U_c + W_c \quad (17.8)$$

suggests that one performs the calculations in the Furry picture [2]. The state vector  $\bar{\Psi}_n(t)$  in this picture is obtained from the Schrödinger state vector  $\Psi_s(t)$  by

$$\bar{\Psi}_n(t) = \exp(i\bar{H}_c t) \Psi_s(t), \quad (17.9)$$

where we have set  $\hbar = 1$ . We recall that in the interaction picture one has [see eq. (13.45)]

$$\Psi_n(t) = \exp(iH_c t) \Psi_s(t). \quad (17.10)$$

The Tomonaga–Schwinger equation for  $\bar{\Psi}_n(t)$  is now given by

$$i \frac{\partial}{\partial t} \bar{\Psi}_n(t) = \bar{W}_c(t) \bar{\Psi}_n(t) \quad (17.11)$$

where

$$\bar{W}_c(t) = \exp(i\bar{H}_c t) W_c \exp(-i\bar{H}_c t). \quad (17.12)$$

The equations (17.11)–(17.12) define the corrections induced by the interactions  $W_c$  to the movement governed by the Hamiltonians  $\bar{H}_c$ . We remark that in the Furry picture the distorted waves  $\chi_n^{(\pm)}$  play the role given to the free waves  $\Phi_n$  in the interaction picture.

Having recognized this important property, we are now prepared to “read off” most of the results of the two-potential formalism. We may define the evolution operators  $\bar{U}_c(t, t_0)$  in the Furry picture from the equation

$$\bar{\Psi}_n(t) = \bar{U}_c(t, t_0) \bar{\Psi}_n(t_0). \quad (17.13)$$

These operators satisfy the integral equations

$$\bar{U}_c(t, t_0) = I - i \int_{t_0}^t \bar{W}_c(t') \bar{U}_c(t', t_0) dt' \quad (17.14a)$$

$$= I + i \int_t^{t_0} \bar{U}_c(t, t') \bar{W}_c(t') dt' \quad (17.14b)$$

and the passage to infinite times may be done as in Chapter 14. We obtain in this way the new Møller operators [compare with eqs. (14.51) and (14.52)]

$$\bar{\Omega}_c^{(\pm)} = \bar{U}_c(0, \mp \infty) A_c \quad (17.15)$$

and

$$\bar{\Omega}_c^{(\pm)\dagger} = A_c \bar{U}_c(\mp \infty, 0) \quad (17.16)$$

such that [3]

$$\Psi_n^{(\pm)} = \bar{\Omega}_c^{(\pm)} \chi_n^{(\pm)} \quad (17.17)$$

and

$$\langle \Psi_n^{(\pm)} | = \langle \chi_n^{(\pm)} | \bar{\Omega}_c^{(\pm)\dagger}. \quad (17.18)$$

We may develop these relations as in Section 14.1 to obtain the formal solutions

$$\Psi_n^{(\pm)} = \chi_n^{(\pm)} + \frac{1}{E_n - H \pm i\varepsilon} W_c \chi_n^{(\pm)}. \quad (17.19a)$$

In particular, we see that in the initial and final arrangement channels one has respectively

$$\Psi_a^{(\pm)} = \chi_a^{(\pm)} + \frac{1}{E_a - H \pm i\varepsilon} W_i \chi_a^{(\pm)} \quad (17.19b)$$

and

$$\Psi_b^{(\pm)} = \chi_b^{(\pm)} + \frac{1}{E_b - H \pm i\varepsilon} W_f \chi_b^{(\pm)}. \quad (17.19c)$$

We note the close analogy between the above formal solutions and those obtained in Section 14.1 from the free waves  $\Phi_n$  [see eqs. (14.66)].



## 17.2. Generalized Lippmann–Schwinger equations

We may now proceed as in Section 16.1 to deduce from eq. (17.19a) the generalized Lippmann–Schwinger equations for  $\Psi_n^{(\pm)}$ . We first note that by using the identities (14.146) and (14.147) one has

$$G^{(\pm)} = \bar{G}_c^{(\pm)} + G^{(\pm)} W_c \bar{G}_c^{(\pm)} \quad (17.20a)$$

and

$$G^{(\pm)} = \bar{G}_c^{(\pm)} + \bar{G}_c^{(\pm)} W_c G^{(\pm)}. \quad (17.20b)$$

Then, from eqs. (17.19a) and (17.20b), we deduce that

$$\Psi_n^{(\pm)} = \chi_n^{(\pm)} + \frac{1}{E_n - \bar{H}_c \pm i\varepsilon} W_c \Psi_n^{(\pm)}. \quad (17.21a)$$

In particular, we have in the initial and final arrangement channels,

$$\Psi_a^{(\pm)} = \chi_a^{(\pm)} + \frac{1}{E_a - \bar{H}_i \pm i\varepsilon} W_i \Psi_a^{(\pm)} \quad (17.21b)$$

and

$$\Psi_b^{(\pm)} = \chi_b^{(\pm)} + \frac{1}{E_b - \bar{H}_f \pm i\varepsilon} W_f \Psi_b^{(\pm)}. \quad (17.21c)$$

It is interesting to obtain eqs. (17.19) and (17.21) directly by formal manipulations, without using the Furry picture arguments given above. To do this we start from the relation (14.66a) for  $\Psi_n^{(\pm)}$ , namely

$$\begin{aligned} \Psi_n^{(\pm)} &= \Phi_n + \frac{1}{E_n - H \pm i\varepsilon} V_c \Phi_n \\ &= \Phi_n + \frac{1}{E_n - H_c - U_c - W_c \pm i\varepsilon} (U_c + W_c) \Phi_n \end{aligned} \quad (17.22)$$

and subtract eq. (17.6) from it. We obtain in this way

$$\begin{aligned} \Psi_n^{(\pm)} &= \chi_n^{(\pm)} + \frac{1}{E_n - H_c - U_c - W_c \pm i\varepsilon} (U_c + W_c) \Phi_n \\ &\quad - \frac{1}{E_n - H_c - U_c \pm i\varepsilon} U_c \Phi_n. \end{aligned} \quad (17.23)$$

We now write the last term on the right-hand side of eq. (17.23) as

$$\frac{1}{E_n - H_c - U_c \pm i\varepsilon} U_c \Phi_n = \frac{1}{(E_n - H_c - U_c - W_c \pm i\varepsilon) + W_c} U_c \Phi_n \quad (17.24)$$

and use the operator identity

$$\frac{1}{A + B} = \frac{1}{A} \left( 1 - B \frac{1}{A + B} \right) \quad (17.25)$$

where

$$A \equiv E_n - H_c - U_c - W_c \pm i\varepsilon, \quad B \equiv W_c. \quad (17.26)$$

Thus eq. (17.23) becomes

$$\begin{aligned} \Psi_n^{(\pm)} &= \chi_n^{(\pm)} + \frac{1}{E_n - H_c - U_c - W_c \pm i\varepsilon} (U_c + W_c) \Phi_n \\ &\quad - \frac{1}{E_n - H_c - U_c - W_c \pm i\varepsilon} U_c \Phi_n \\ &\quad + \frac{1}{E_n - H_c - U_c - W_c \pm i\varepsilon} W_c \frac{1}{E_n - H_c - U_c \pm i\varepsilon} U_c \Phi_n. \end{aligned} \quad (17.27)$$

Simplifying the right-hand side and using the fact that

$$\frac{1}{E_n - H_c - U_c \pm i\varepsilon} U_c \Phi_n = \chi_n^{(\pm)} - \Phi_n \quad (17.28)$$

we find that

$$\Psi_n^{(\pm)} = \chi_n^{(\pm)} + \frac{1}{E_n - H_c - U_c - W_c \pm i\varepsilon} W_c \chi_n^{(\pm)} \quad (17.29)$$

or

$$\Psi_n^{(\pm)} = \chi_n^{(\pm)} + \frac{1}{E_n - H \pm i\varepsilon} W_c \chi_n^{(\pm)} \quad (17.30)$$

which is precisely eq. (17.19a). The generalized Lippmann-Schwinger equations (17.21) follow by using eq. (17.20b).

### 17.3. The two-potential formulae

We now turn to the calculation of the (on-the-energy-shell) transition matrix element  $\langle b | \mathcal{T} | a \rangle$ . It is given by the integral representations (14.157), namely

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)} | V_i | \Phi_a \rangle. \quad (17.31)$$

Thus, for the two-potential problem considered here, we have

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | U_f + W_f | \Psi_a^{(+)} \rangle \quad (17.32a)$$

and

$$\langle b | \mathcal{T} | a \rangle = \langle \Psi_b^{(-)} | U_i + W_i | \Phi_a \rangle. \quad (17.32b)$$

Let us focus our attention on eq. (17.32a) and introduce the distorted waves in this formula. From eq. (17.6) we deduce that

$$\chi_b^{(-)} = \Phi_b + \frac{1}{E_b - H_f - i\varepsilon} U_f \Phi_b \quad (17.33)$$

so that

$$\langle \Phi_b | = \langle \chi_b^{(-)} | - \langle \Phi_b | U_f \frac{1}{E_b - \bar{H}_f + i\varepsilon} \quad (17.34)$$

and therefore

$$\begin{aligned} \langle b | \mathcal{T} | a \rangle &= \langle \Phi_b | U_f | \Psi_a^{(+)} \rangle + \langle \chi_b^{(-)} | W_f | \Psi_a^{(+)} \rangle \\ &\quad - \left\langle \Phi_b \left| U_f \frac{1}{E_b - \bar{H}_f + i\varepsilon} W_f \right| \Psi_a^{(+)} \right\rangle. \end{aligned} \quad (17.35)$$

The third term on the right-hand side of eq. (17.35) may be transformed by making use of eqs. (14.66b) and (17.34) so that on the energy shell ( $E = E_a = E_b$ )

$$\begin{aligned} \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \right| \Psi_a^{(+)} \right\rangle &= \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \right| \Phi_a \right\rangle \\ &\quad + \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle \end{aligned} \quad (17.36)$$

or

$$\begin{aligned} \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \right| \Psi_a^{(+)} \right\rangle &= \langle \chi_b^{(-)} | W_f | \Phi_a \rangle - \langle \Phi_b | W_f | \Phi_a \rangle \\ &\quad + \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle. \end{aligned} \quad (17.37)$$

Furthermore, from the operator identity

$$\frac{1}{B}(B - A)\frac{1}{A} = \frac{1}{A} - \frac{1}{B}$$

with  $A \equiv E - H + i\varepsilon$  and  $B \equiv E - \bar{H}_f + i\varepsilon$ , we find that

$$\begin{aligned} &\left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle \\ &= \left\langle \Phi_b \left| U_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle - \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} V_i \right| \Phi_a \right\rangle \end{aligned} \quad (17.38)$$

or, using eqs. (14.66b) and (17.34),

$$\begin{aligned} \left\langle \Phi_b \left| U_f \frac{1}{E - \bar{H}_f + i\varepsilon} W_f \frac{1}{E - H + i\varepsilon} V_i \right| \Phi_a \right\rangle &= \langle \Phi_b | U_f | \Psi_a^{(+)} \rangle \\ &\quad - \langle \Phi_b | U_f | \Phi_a \rangle - \langle \chi_b^{(-)} | V_i | \Phi_a \rangle + \langle \Phi_b | V_i | \Phi_a \rangle. \end{aligned} \quad (17.39)$$

Making use of the results (17.37) and (17.39) in eq. (17.35) and taking into account the fact that on the energy shell

$$\langle \Phi_b | U_f + W_f | \Phi_a \rangle = \langle \Phi_b | V_f | \Phi_a \rangle = \langle \Phi_b | V_i | \Phi_a \rangle \quad (17.40)$$

we find that

$$\langle b | \mathcal{T} | a \rangle = \langle \chi_b^{(-)} | V_i - W_f | \Phi_a \rangle + \langle \chi_b^{(-)} | W_f | \Psi_a^{(+)} \rangle. \quad (17.41)$$

A similar reasoning, starting from eq. (17.32b) leads to the "symmetric" formula

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | V_f - W_i | \chi_a^{(+)} \rangle + \langle \Psi_b^{(-)} | W_i | \chi_a^{(+)} \rangle. \quad (17.42)$$

The results (17.41) and (17.42) are the *two-potential formulae of Gell-Mann and Goldberger* [1] (see also ref. [4]). They simplify when

$$H_i = H_f = H_d; \quad V_i = V_f = V_d; \quad U_i = U_f = U; \quad W_i = W_f = W \quad (17.43)$$

so that  $V_d = U + W$  and  $H = H_d + V_d = H_d + U + W$ . In this case eqs. (17.41) and (17.42) yield the relations

$$\langle b | \mathcal{T} | a \rangle = \langle \chi_b^{(-)} | U | \Phi_a \rangle + \langle \chi_b^{(-)} | W | \Psi_a^{(+)} \rangle \quad (17.44)$$

or

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | U | \chi_a^{(+)} \rangle + \langle \Psi_b^{(-)} | W | \chi_a^{(+)} \rangle \quad (17.45)$$

which are known as *Watson's theorem* [5].

An interesting physical interpretation of these formulae may be found in the following way. If we start for example from eq. (17.44) and recall that

$$\Psi_a^{(+)} = \chi_a^{(+)} + \frac{1}{E_a - H + i\epsilon} W \chi_a^{(+)} \quad (17.46)$$

we may write the transition matrix element (on the energy shell) as

$$\begin{aligned} \langle b | \mathcal{T} | a \rangle = & \langle \chi_b^{(-)} | U | \Phi_a \rangle \\ & + \left\langle \chi_b^{(-)} \left| W + W \frac{1}{E - H_d - U - W} W \right| \chi_a^{(+)} \right\rangle. \end{aligned} \quad (17.47)$$

The first term on the right-hand side of eq. (17.47) clearly describes the transition due to the interaction  $U$  alone. The second term has also the structure of a transition matrix element induced by the potential  $W$  [see eq. (14.170)], *but between the distorted waves*  $\chi_a^{(+)}$  and  $\chi_b^{(-)}$ . Furthermore the corresponding Hamiltonian is evidently  $H_d + U + W$  and not simply  $H_d + W$ . This term may therefore be interpreted as a transition matrix element describing *the scattering by the potential  $W$  in the presence of the interaction  $U$ .*

Another interesting simplification of the two-potential formulae (17.41) and (17.42) occurs when the *distorting potentials*  $U_i$  and  $U_f$  *cannot induce the transition*  $a \rightarrow b$  *considered*. This may happen for example if the interactions

$U_i$  and  $U_f$  only generate elastic scattering and the transition  $a \rightarrow b$  is an inelastic process or a rearrangement collision. In this case the first term on the right-hand side of eqs. (17.41)–(17.42) vanishes so that

$$\langle b|\mathcal{T}|a\rangle = \langle \chi_b^{(-)}|W_f|\Psi_a^{(+)}\rangle = \langle \Psi_b^{(-)}|W_i|\chi_a^{(+)}\rangle \quad (17.48)$$

in direct analogy with the “free waves” formulae (14.157).

### 17.4. Distorted wave Born series

Let us continue to treat exactly the potentials  $U_i$  and  $U_f$  but elect to use perturbation theory to handle the interactions  $W_i$  and  $W_f$ . We generate in this way the *distorted wave Born series* for the wave functions and the transition matrix element.

To see how this can be done, we return to the Lippmann–Schwinger equations (17.21b) and (17.21c) which we solve by iteration, starting from the distorted waves  $\chi_a^{(\pm)}$  and  $\chi_b^{(\pm)}$  as our first approximation. Thus, writing

$$\Psi_a^{(+)} \simeq \chi_a^{(+)}; \quad \Psi_b^{(-)} \simeq \chi_b^{(-)} \quad (17.49)$$

and substituting in eqs. (17.41) and (17.42) we obtain the first term of the distorted wave Born series for the transition matrix element, namely the *distorted wave Born approximation* (DWBA)

$$\langle b|\mathcal{T}|a\rangle_{\text{DWBA}} = \langle \chi_b^{(-)}|V_i - W_f|\Phi_a\rangle + \langle \chi_b^{(-)}|W_f|\chi_a^{(+)}\rangle \quad (17.50)$$

or

$$\langle b|\mathcal{T}|a\rangle_{\text{DWBA}} = \langle \Phi_b|V_f - W_i|\chi_a^{(+)}\rangle + \langle \chi_b^{(-)}|W_i|\chi_a^{(+)}\rangle. \quad (17.51)$$

Although formally different, the two expressions (17.50) and (17.51) for the DWBA transition matrix element are easily seen to be equivalent. They are better approximations to the exact  $T$ -matrix element than the expressions

$$\langle b|\mathcal{T}|a\rangle \simeq \langle \chi_b^{(-)}|V_i - W_f|\Phi_a\rangle + \langle \chi_b^{(-)}|W_f|\Phi_a\rangle \quad (17.52)$$

or

$$\langle b|\mathcal{T}|a\rangle \simeq \langle \Phi_b|V_f - W_i|\chi_a^{(+)}\rangle + \langle \Phi_b|W_i|\chi_a^{(+)}\rangle \quad (17.53)$$

which would be obtained by using directly the approximations (17.49) in the original integral representations (17.31). Indeed, by comparing the two approximations (17.50) and (17.52) with the exact expression (17.41), we see that in eq. (17.50) the exact state vector  $\Psi_a^{(+)}$  has been replaced by  $\chi_a^{(+)}$  while in eq. (17.52) it is replaced by  $\Phi_a$ . Now, if the effect of  $W_i$  is sufficiently weak, the distorted wave  $\chi_a^{(+)}$  should be “closer” to the exact solution  $\Psi_a^{(+)}$  than is the free wave  $\Phi_a$ , so that the DWBA approximation should be preferred to the approximation (17.52). Similarly the DWBA expression (17.51) is intrinsically superior to the approximation (17.53) provided that  $W_f$  may be treated as a perturbation.

If the potentials  $U_i$  and  $U_f$  cannot induce the transition  $a \rightarrow b$ , we may start from the exact formulae (17.48) to obtain the DWBA approximation

$$\langle b|\mathcal{T}|a\rangle_{\text{DWBA}} = \langle \chi_b^{(-)}|W_i|\chi_a^{(+)}\rangle = \langle \chi_b^{(-)}|W_f|\chi_a^{(+)}\rangle \quad (17.54)$$

whose analogy with the first Born approximation for free waves [eq. (16.30)] is obvious.

A simple, but physically appealing interpretation of eq. (17.54) may be given. Let us imagine for example that the transition  $a \rightarrow b$  is a binary rearrangement collision of the type  $A + B \rightarrow C + D$  (see Fig. 17.1).

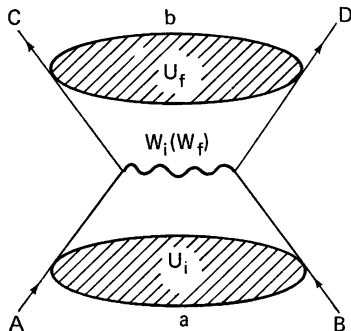


Fig. 17.1. A diagrammatic interpretation of the DWBA matrix element (17.54).

As shown in this figure, we see that the two particles A and B feel the interaction  $U_i$  (embodied in  $\chi_a^{(+)}$ ) in the initial channel, then interact *once* through  $W_i$  (or  $W_f$ ), and finally interact through the potential  $U_f$  (contained in  $\chi_b^{(-)}$ ) while emerging from the collision. It is important to note that  $U_i$  and  $U_f$  are treated exactly so that the particles can interact repeatedly through  $U_i$  and  $U_f$ , while the potentials  $W_i$  or  $W_f$  are only allowed to act *once* in the DWBA approximation.

Higher order terms in the distorted waves Born series may be written down in the same way as for the Born series in Section 16.2. Thus, solving eqs. (17.20) and (17.21) by iteration, we obtain respectively the distorted wave Born series for the full Green's operators  $G^{(\pm)}$  and the state vectors  $\Psi_n^{(\pm)}$ , namely

$$G^{(\pm)} = \bar{G}_c^{(\pm)} + \bar{G}_c^{(\pm)}W_c\bar{G}_c^{(\pm)} + \bar{G}_c^{(\pm)}W_c\bar{G}_c^{(\pm)}W_c\bar{G}_c^{(\pm)} + \cdots \quad (17.55)$$

and

$$\Psi_n^{(\pm)} = \chi_n^{(\pm)} + \bar{G}_c^{(\pm)}W_c\chi_n^{(\pm)} + \bar{G}_c^{(\pm)}W_c\bar{G}_c^{(\pm)}W_c\chi_n^{(\pm)} + \cdots \quad (17.56)$$

The corresponding distorted wave Born series for the  $T$  matrix element  $\langle b|\mathcal{T}|a\rangle$  are obtained by replacing  $|\chi_a^{(+)}\rangle$  and  $\langle\chi_b^{(-)}|$  by their distorted wave Born series in the two-potential formulae (17.41) and (17.42). Completely similar formulae may of course be written down for the reduced  $T$  matrix element  $T_{ba}$ .

The DWBA formula (17.54) has been used extensively to study atomic [6] and nuclear [7] collisions. It also provided an intuitive starting point for various high-energy absorption models [8–10]. When the conditions of validity of the eikonal approximation are satisfied (see Section 9.1), the distorted waves  $\chi_a^{(+)}$  and  $\chi_b^{(-)}$  appearing in eq. (17.54) may be replaced by the corresponding eikonal wave functions. The evaluation of the matrix elements (17.54) is then considerably simplified. This *eikonal DWBA approximation* has been applied to various high-energy processes [9, 11, 12] and more recently to atomic collisions [13–15].

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## **PART IV**

## **APPLICATIONS**

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## Two-Body Collisions

In this chapter we shall consider scattering processes in which two “elementary” [1] particles are present in both the initial and final states. For spinless particles and in the non-relativistic case this problem reduces to the simple one of potential scattering which we studied in detail in Part II. We shall now use the theory of Part III to extend this treatment to the case of relativistic collisions and (or) two-body collisions involving particles with spin.

We begin by considering in Section 18.1 the simple case of *central forces*. Starting from the Heitler equation we perform a partial wave analysis and obtain the explicit expressions of the  $S$ ,  $T$  and  $K$ -matrices in terms of phase shifts. Off-shell extensions and unitarity relations for partial wave scattering matrices are also discussed. The next two sections are concerned with *non-central interactions*. The basic techniques involved are developed in Section 18.2. They are applied in Section 18.3 to the scattering of spin zero by spin one-half particles. Finally, in Section 18.4, we use the Regge pole ideas exposed in Section 11.4 to give a brief, phenomenological account of two-body hadronic collisions at high energies.

### 18.1. Central forces

Let us consider the scattering in the C.M. system of two particles A and B, having respectively masses  $m_A$  and  $m_B$ , spins  $S_A$  and  $S_B$  and C.M. energies  $E_A$  and  $E_B$ . Before the scattering, the two particles have the respective momenta  $\mathbf{p}_A = \mathbf{p}_1$  and  $\mathbf{p}_B = -\mathbf{p}_1$ , where  $\mathbf{p}_1$  is the initial relative momentum. We shall denote by  $\mathbf{k}_1$  the corresponding initial relative wave vector, such

that  $p_i = \hbar k_i$ . The total initial C.M. energy is given by

$$E_a = E_A + E_B = c[(m_A^2 c^2 + p_i^2)^{1/2} + (m_B^2 c^2 + p_i^2)^{1/2}] \\ = c[(m_A^2 c^2 + \hbar^2 k_i^2)^{1/2} + (m_B^2 c^2 + \hbar^2 k_i^2)^{1/2}] \quad (18.1)$$

with  $p_i = |p_i|$  and  $k_i = |k_i|$ .

After the scattering the two particles will have the respective C.M. momenta  $p_f$  and  $-p_f$ , the corresponding wave vectors being  $k_f$  and  $-k_f$  (with  $p_f = \hbar k_f$ ). Their total final C.M. energy is given by

$$E_b = c[(m_A^2 c^2 + p_f^2)^{1/2} + (m_B^2 c^2 + p_f^2)^{1/2}] \\ = c[(m_A^2 c^2 + \hbar^2 k_f^2)^{1/2} + (m_B^2 c^2 + \hbar^2 k_f^2)^{1/2}]. \quad (18.2)$$

Energy conservation therefore requires that  $p_i = p_f$  (or  $k_i = k_f$ ).

We shall assume for the moment [2] that the internal states of the colliding particles will not be affected by the scattering, except perhaps for certain spin modifications which we shall specify shortly. Let us denote by  $S_A(S_A + 1)\hbar^2$  and  $v_A\hbar$  the initial eigenvalues of the operators  $S_A^2$  and  $S_A \cdot \hat{u}$ , where  $\hat{u}$  is the unit vector along a given axis. The final eigenvalues of these operators (after the collision) will be denoted by  $S'_A(S'_A + 1)\hbar^2$  and  $v'_A\hbar$ . We adopt a similar definition for the eigenvalues  $S_B(S_B + 1)\hbar^2$ ,  $v_B\hbar$  and  $S'_B(S'_B + 1)\hbar^2$ ,  $v'_B\hbar$  of the operators  $S_B^2$  and  $S_B \cdot \hat{u}$ . Finally, if  $S = S_A + S_B$  is the total spin of the two particles, we shall write the eigenvalues of the operators  $S^2$  and  $S \cdot \hat{u}$  before and after the collision as  $S(S + 1)\hbar^2$ ,  $v\hbar$  and  $S'(S' + 1)\hbar^2$ ,  $v'\hbar$ .

In this section we shall consider two-body collisions in which the interaction  $V$  between the colliding particles is *central*. That is,

$$[S, H] = 0 \quad (18.3)$$

where  $H$  is the total Hamiltonian of the system. We may also write

$$\langle S' | V | S \rangle = \delta_{SS'} V^{(S)} \quad (18.4)$$

where  $V^{(S)}$  is the interaction occurring in the state of total spin  $S$ . The total angular momentum in the C.M. system is evidently

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \quad (18.5)$$

where the orbital angular momentum  $\mathbf{L}$  is given by

$$\mathbf{L} = \mathbf{r}_A \times \mathbf{p}_i + \mathbf{r}_B \times (-\mathbf{p}_i) = (\mathbf{r}_A - \mathbf{r}_B) \times \mathbf{p}_i \\ = \mathbf{r} \times \mathbf{p}_i. \quad (18.6)$$

Here  $\mathbf{r}_A$  and  $\mathbf{r}_B$  are the coordinates of the particles A and B and  $\mathbf{r} = \mathbf{r}_A - \mathbf{r}_B$ . We shall assume that the Hamiltonian  $H$  is rotational invariant so that [see eq. (16.174)]

$$[\mathbf{J}, H] = 0. \quad (18.7)$$

Then, from eqs. (18.3), (18.5) and (18.7) we deduce that

$$[\mathbf{L}, H] = 0. \quad (18.8)$$

Now, according to eqs. (16.184), we see that the condition (18.3) implies that the reduced transition matrix element  $T_{ba}$  and its off-the-energy-shell extensions  $T_{ba}^{(\pm)}(E_b, E_a)$  and  $T_{ba}(E_b, E_a, E)$  are diagonal in  $S$  and  $v$  and also independent of  $v$ . Moreover, since the orbital angular momentum  $L$  generates the infinitesimal rotations in configuration or momentum space, the condition (18.8) means that the only dependence of the  $T$ -matrix element on the initial and final C.M. wave vectors  $k_i$  and  $k_f$  will be in the form of scalar products of  $k_i$  and  $k_f$ , namely  $k_i^2$  (or  $k_i$ ),  $k_f^2$  (or  $k_f$ ) and  $k_i \cdot k_f$ . We may thus write the on-the-energy-shell reduced  $T$ -matrix element as

$$T_{ba} \equiv \langle k_f, S', v' | T | k_i, S, v \rangle = \delta_{SS'} \delta_{vv'} T^{(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f), \quad k_i = k_f = k. \quad (18.9a)$$

Similarly, the off-the-energy shell matrix elements  $T_{ba}^{(\pm)}(E_b, E_a)$  are given by

$$T_{ba}^{(\pm)} \equiv \langle k_f, S', v' | T^{(\pm)} | k_i, S, v \rangle = \delta_{SS'} \delta_{vv'} T^{(\pm)(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f), \quad k_i \neq k_f \quad (18.9b)$$

while the completely off-the-energy shell  $T$ -matrix element  $T_{ba}(E_b, E_a, E)$  is such that

$$T_{ba}(E_b, E_a, E) \equiv \langle k_f, S', v' | T(E) | k_i, S, v \rangle = \delta_{SS'} \delta_{vv'} T^{(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f, k), \quad k \neq k_i \neq k_f. \quad (18.9c)$$

We note that the only spin modifications allowed by central interactions are changes in the individual spin *orientations* of the particles (i.e. in the individual azimuthal components  $v_A$  and  $v_B$ ) satisfying the condition  $v = v'$  (or  $v_A + v_B = v'_A + v'_B$ ).

A particular case of central forces arises when the interaction  $V$  is totally *spin-independent*. Then one has

$$[S_A, H] = [S_B, H] = 0 \quad (18.10)$$

and the quantity  $V^{(S)}$  appearing in eq. (18.4) is obviously independent of the total spin  $S$ . The reduced on-the-energy shell  $T$ -matrix element is then given by

$$T_{ba} \equiv \langle k_f, v'_A, v'_B | T | k_i, v_A, v_B \rangle = \delta_{v_A v'_A} \delta_{v_B v'_B} T(k, k, \hat{k}_i \cdot \hat{k}_f), \quad k = k_i = k_f \quad (18.11)$$

and similar expressions may be written for the off-shell quantities  $T_{ba}^{(\pm)}(E_b, E_a)$  and  $T_{ba}(E_b, E_a, E)$ . Hence the only allowed transitions are of the type  $(v_A, v_B) \rightarrow (v_A, v_B)$ . The stationary solutions of the (time-independent) Schrödinger equation of the system are of the form

$$\Psi(\mathbf{r}, s_A, s_B) = \psi(\mathbf{r}) \chi_{v_A}(s_A) \chi_{v_B}(s_B) \quad (18.12)$$

where  $\chi_{v_A}(s_A)$  and  $\chi_{v_B}(s_B)$  are the spin eigenvectors of the two colliding particles, while  $s_A$  and  $s_B$  are the corresponding (discrete) spin variables. For the more general case of central forces we have instead

$$\Psi(\mathbf{r}, s_A, s_B) = \psi(\mathbf{r}) \chi_{Sv}(s_A, s_B) \quad (18.13)$$

with

$$\chi_{Sv}(s_A, s_B) = \sum_{\substack{v_A, v_B \\ (v_A + v_B = v)}} \langle S_A S_B v_A v_B | S v \rangle \chi_{v_A}(s_A) \chi_{v_B}(s_B) \quad (18.14)$$

where  $\langle S_A S_B v_A v_B | S v \rangle$  is a vector addition or Clebsch-Gordan (C.G.) coefficient [3].

Let us now consider the Lippmann-Schwinger equation for the off-the-energy shell  $T$ -matrix elements  $T_{ba}^{(+)}$ . We may use eq. (16.20a) to write in the  $\{S, v\}$  representation

$$\begin{aligned} \langle k_f, S', v' | T^{(+)} | k_i, S, v \rangle &= \langle k_f, S', v' | V | k_i, S, v \rangle \\ &+ \sum_{S'', v''} \int dk'' \frac{\langle k_f, S', v' | V | k'', S'', v'' \rangle \langle k'', S'', v'' | T^{(+)} | k_i, S, v \rangle}{E_a(k_i) - E(k'') + i\epsilon} \end{aligned} \quad (18.15)$$

where  $k''$  is an intermediate wave vector and  $E(k'')$  the corresponding energy. Using eqs. (18.4) and (18.9) we find that

$$\begin{aligned} T^{(+)(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f) &= V^{(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f) \\ &+ \int dk' \frac{V^{(S)}(k_f, k', \hat{k}' \cdot \hat{k}_f) T^{(+)(S)}(k', k_i, \hat{k}_i \cdot \hat{k}')}{E_a(k_i) - E(k') + i\epsilon} \end{aligned} \quad (18.16a)$$

where we have now written  $k'$  for the intermediate wave vector. For spin-independent interactions we may use eq. (18.11) and the fact that  $V$  is independent of  $S$  to obtain a similar equation, but where the index  $S$  has disappeared. In the same way, one also obtains from eq. (16.20b) the Lippmann-Schwinger equation

$$\begin{aligned} T^{(-)(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f) &= V^{(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f) \\ &+ \int dk' \frac{T^{(-)(S)}(k_f, k', \hat{k}' \cdot \hat{k}_f) V^{(S)}(k', k_i, \hat{k}_i \cdot \hat{k}')}{E_b(k_f) - E(k') + i\epsilon}. \end{aligned} \quad (18.16b)$$

We recall that the on-the-energy-shell  $T$ -matrix must be obtained from either version of eq. (18.16) by first solving it and then setting  $E_a = E_b$ .

We shall also need expressions for the  $K$ -matrix elements. Because the  $K$ -operator [see eq. (16.85a)]

$$K = V + VP \left( \frac{1}{E - H_0} \right) K \quad (18.17)$$

commutes with  $L$  and  $S$  in the case of central forces, we also have

$$\begin{aligned} K_{ba} &\equiv \langle k_f, S', v' | K | k_i, S, v \rangle = \delta_{SS'} \delta_{vv'} K^{(S)}(k, k, \hat{k}_i \cdot \hat{k}_f), \\ k &= k_i = k_f \end{aligned} \quad (18.18a)$$

for the on-the-energy-shell  $K$ -matrix elements. Similar expressions hold for the off-shell quantities  $K_{ba}^{(\pm)}(E_b, E_a)$  and  $K_{ba}(E_b, E_a, E)$ . That is,

$$\begin{aligned} K_{ba}^{(\pm)} &\equiv \langle k_f, S', v' | K^{(\pm)} | k_i, S, v \rangle = \delta_{SS'} \delta_{vv'} K^{(\pm)(S)}(k_f, k_i, \hat{k}_i \cdot \hat{k}_f), \\ k_i &\neq k_f \end{aligned} \quad (18.18b)$$

and

$$K_{ba}(E_b, E_a, E) \equiv \langle \mathbf{k}_f, S', v' | K(E) | \mathbf{k}_i, S, v \rangle = \delta_{SS'} \delta_{vv'} K^{(S)}(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f, k),$$

$$k \neq k_i \neq k_f. \quad (18.18c)$$

For spin-independent forces, where the operator  $K$  commutes with  $L$ ,  $S_A$  and  $S_B$ , one has

$$K_{ba} \equiv \langle \mathbf{k}_f, v'_A, v'_B | K | \mathbf{k}_i, v_A, v_B \rangle = \delta_{v_A v'_A} \delta_{v_B v'_B} K(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f),$$

$$k = k_i = k_f \quad (18.19)$$

with similar expressions for  $K_{ba}^{(\pm)}(E_b, E_a)$  and  $K_{ba}(E_b, E_a, E)$ .

Using eq. (16.89a) we may then write in the  $(S, v)$  representation

$$K^{(+)(S)}(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) = V^{(S)}(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f)$$

$$+ P \int d\mathbf{k}' \frac{V^{(S)}(k_f, k', \hat{\mathbf{k}}_f \cdot \hat{\mathbf{k}}') K^{(+)(S)}(k', k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}')}{E_a(k_i) - E(k')}. \quad (18.20)$$

A similar equation – with no spin index  $S$  – holds for spin-independent forces.

Let us now write the Heitler equation, which connects the  $T$  and  $K$  matrices on the energy shell. From eq. (16.93a) we first write on the energy-momentum shell

$$T_{ba} = K_{ba} - i\pi \sum_n \delta(E - E_n) K_{bn} T_{na}. \quad (18.21)$$

Then, using eqs. (18.9) and (18.18) we find in the  $\{S, v\}$  representation that

$$T^{(S)}(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) = K^{(S)}(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) \quad (18.22)$$

$$- i\pi \int d\Omega' \int_0^\infty dk' k'^2 K^{(S)}(k, k', \hat{\mathbf{k}}_f \cdot \hat{\mathbf{k}}') \delta[E(k) - E(k')] T^{(S)}(k', k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}')$$

where  $d\Omega'$  is an element of solid angle in which the vector  $\mathbf{k}'$  is pointing.

In order to perform the integration on the variable  $k'$  we introduce as in Section 15.2 the density of states per unit energy  $\rho(E)$  such that

$$\rho(E) dE = k^2 dk \quad (18.23)$$

and therefore

$$\rho(E) = k^2 dk/dE. \quad (18.24)$$

We then obtain at once

$$T^{(S)}(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) = K^{(S)}(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f)$$

$$- i\pi \rho(E) \int d\Omega' K^{(S)}(k, k, \hat{\mathbf{k}}_f \cdot \hat{\mathbf{k}}') T^{(S)}(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}'). \quad (18.25)$$

A similar equation holds for the case of spin-independent interactions with  $T$  and  $K$  matrices independent of the spin index  $S$ . In what follows we shall simplify the notation by omitting the index  $S$ , so that we shall formally

treat central and spin-independent interactions on the same footing. It should be remembered, however, that a *given* value of  $S$  is always implicit when  $T$  and  $K$  actually depend on  $S$ .

We now proceed to solve eq. (18.25) by expanding the  $T$  and  $K$  matrices in spherical harmonics. Defining  $\cos \theta = \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f$ , we write

$$\begin{aligned} T(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) &= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} T_l(k) P_l(\cos \theta) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} T_l(k) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \quad k_i = k_f = k \end{aligned} \quad (18.26a)$$

and more generally,

$$T^{(\pm)}(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} T_l^{(\pm)}(k_f, k_i) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \quad k_i \neq k_f \quad (18.26b)$$

$$\begin{aligned} T(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f, k) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} T_l(k_f, k_i, k) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \\ &k \neq k_i \neq k_f. \end{aligned} \quad (18.26c)$$

Similarly,

$$K(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} K_l(k) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \quad k = k_i = k_f \quad (18.27a)$$

$$K^{(\pm)}(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} K_l^{(\pm)}(k_f, k_i) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \quad k_i \neq k_f \quad (18.27b)$$

and

$$\begin{aligned} K(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f, k) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} K_l(k_f, k_i, k) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i), \\ &k \neq k_i \neq k_f \end{aligned} \quad (18.27c)$$

where we recall that [see eq. (16.24b)]

$$T_l(k) = T_l^{(\pm)}(k, k) \quad (18.28)$$

and we have also defined

$$K_l(k) = K_l^{(\pm)}(k, k) \quad (18.29)$$

on the energy shell. Since the  $K$ -matrix is Hermitian and the Legendre polynomials are real, we note that

$$K_l(k) = K_l^*(k) \quad (18.30)$$

so that  $K_l(k)$  is a *real* quantity. Inserting the expansions (18.26a) and (18.27a) in eq. (18.25) we find by using the orthonormality of the spherical harmonics that

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) [T_l(k) - K_l(k) + i\pi\rho(E)K_l(k)T_l(k)] = 0. \quad (18.31)$$



Therefore we have reduced the Heitler equation to the set of algebraic equations

$$T_l(k) = K_l(k) - i\pi\rho(E)K_l(k)T_l(k) \quad (18.32)$$

which yield

$$T_l(k) = \frac{K_l(k)}{1 + i\pi\rho(E)K_l(k)} \quad (18.33)$$

and also

$$K_l(k) = \frac{T_l(k)}{1 - i\pi\rho(E)T_l(k)}. \quad (18.34)$$

Because  $K_l(k)$  is a *real* number, it is a natural candidate for a simple parametrization. Let us write

$$K_l(k) = -\frac{1}{\pi\rho(E)} \tan \delta_l(k) \quad (18.35)$$

so that

$$T_l(k) = -\frac{1}{\pi\rho(E)} \exp\{i\delta_l(k)\} \sin \delta_l(k). \quad (18.36)$$

We shall call the quantities  $\delta_l(k)$  the *phase shifts*. It is a simple matter to show that in the simple case of non-relativistic potential scattering the phase shifts defined by eq. (18.35) agree (modulo  $\pi$ ) with those introduced in Chapter 4. To see this we first use eqs. (15.50) and (15.51) together with  $k_i = k_f = k$  and  $\rho(E) = k^2 dk/dE$  to write the scattering amplitude as

$$f_{ba} = -(2\pi)^2(k dk/dE)T_{ba} \quad (18.37)$$

for both non-relativistic and relativistic collisions. We have adopted here the phase convention  $\phi = \pi$  [see eqs. (15.52)–(15.54)]. For general (spin-dependent) central forces we may obtain from eq. (18.37) the scattering amplitude corresponding to a *given* value of  $S$ . It is

$$f^{(S)} = -(2\pi)^2(k dk/dE) T^{(S)}(k, k, \hat{k}_i \cdot \hat{k}_f). \quad (18.38)$$

For spin-independent interactions we obviously have

$$f = -(2\pi)^2(k dk/dE) T(k, k, \hat{k}_i \cdot \hat{k}_f). \quad (18.39)$$

If we insert in this last equation the expansion (18.26a) and use eq. (18.36) together with eq. (18.24) we obtain

$$f = \frac{4\pi}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \exp\{i\delta_l(k)\} \sin \delta_l(k) Y_{lm}(\hat{k}_f) Y_{lm}^*(\hat{k}_i). \quad (18.40)$$

The “addition theorem” of the spherical harmonics, namely [see eq. (B.39) of Appendix B]

$$P_l(\cos \theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y_{lm}(\hat{k}_f) Y_{lm}^*(\hat{k}_i), \quad \cos \theta = \hat{k}_i \cdot \hat{k}_f \quad (18.41)$$

then allows us to write eq. (18.40) in the form

$$f = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp\{i\delta_l(k)\} \sin \delta_l(k) P_l(\cos \theta) \quad (18.42)$$

which is precisely eq. (4.66). It is important to note that this relation, which holds for spin-independent forces, is valid for relativistic as well as non-relativistic two-body collisions. For spin-dependent central forces we obtain in the same way

$$f^{(S)} = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp\{i\delta_l^{(S)}(k)\} \sin \delta_l^{(S)}(k) P_l(\cos \theta) \quad (18.43)$$

where we have now written explicitly the spin label  $S$  in  $\delta_l^{(S)}$ .

Let us return for a moment to the set of algebraic partial wave Heitler equations (18.32) involving the "on-shell" quantities  $T_l(k)$  and  $K_l(k)$ . It is possible to generalize these equations by starting from the operator form (16.94) of the Heitler equations, inserting a complete set of free states and decomposing the off-the-energy shell matrix elements in partial waves [see eqs. (18.26) and (18.27)]. This yields the set of algebraic equations

$$T_l(k_f, k_i, k) = K_l(k_f, k_i, k) - i\pi\rho(E)K_l^{(+)}(k_f, k)T_l^{(-)}(k, k_i) \quad (18.44a)$$

and

$$T_l(k_f, k_i, k) = K_l(k_f, k_i, k) - i\pi\rho(E)T_l^{(+)}(k_f, k)K_l^{(-)}(k, k_i). \quad (18.44b)$$

But from eq. (18.44a) and the fact that  $T_l^{(-)}(k, k_i) = T_l(k, k_i, k)$  we also deduce that

$$\begin{aligned} T_l^{(-)}(k, k_i) &= K_l(k, k_i, k) - i\pi\rho(E)K_l^{(+)}(k, k)T_l^{(-)}(k, k_i) \\ &= K_l^{(-)}(k, k_i) - i\pi\rho(E)K_l(k)T_l^{(-)}(k, k_i) \end{aligned}$$

and therefore

$$T_l^{(-)}(k, k_i) = \frac{K_l^{(-)}(k, k_i)}{1 + i\pi\rho(E)K_l(k)}. \quad (18.45a)$$

Similarly,

$$T_l^{(+)}(k_f, k) = \frac{K_l^{(+)}(k_f, k)}{1 + i\pi\rho(E)K_l(k)}. \quad (18.45b)$$

Substituting eqs. (18.45) into eqs. (18.44) we then obtain the generalized partial wave Heitler equations [4, 5]

$$T_l(k_f, k_i, k) = K_l(k_f, k_i, k) - i\pi\rho(E) \frac{K_l^{(+)}(k_f, k)K_l^{(-)}(k, k_i)}{1 + i\pi\rho(E)K_l(k)}. \quad (18.46)$$

Having obtained the expressions (18.35) and (18.36) for the on-shell  $K$  and  $T$  matrices in terms of the phase shifts, we now proceed to perform the corresponding decomposition of the  $S$ -matrix into states of well defined orbital angular momentum. To this end, we first write the  $S$ -matrix elements as

$$S_{\text{pa}} = \langle \mathbf{k}_f, S', v' | S | \mathbf{k}_i, S, v \rangle = \langle \mathbf{k}_f | S | \mathbf{k}_i \rangle^{(S)} \delta_{SS'} \delta_{vv'}. \quad (18.47)$$

for central forces, and

$$S_{ba} = \langle \mathbf{k}_f, v'_A, v'_B | S | \mathbf{k}_i, v_A, v_B \rangle = \langle \mathbf{k}_f | S | \mathbf{k}_i \rangle \delta_{v_A v'_A} \delta_{v_B v'_B} \quad (18.48)$$

for spin-independent forces. In what follows we shall omit the superscript ( $S$ ) appearing on the right-hand side of eq. (18.47). Moreover,

$$\begin{aligned} \langle \mathbf{k}_f | S | \mathbf{k}_i \rangle &= \delta(\mathbf{k}_f - \mathbf{k}_i) - 2\pi i \delta[E(k_i) - E(k_f)] \langle \mathbf{k}_f | T | \mathbf{k}_i \rangle \\ &= \delta(\mathbf{k}_f - \mathbf{k}_i) - 2\pi i \delta[E(k_i) - E(k_f)] T(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f). \end{aligned} \quad (18.49)$$

We have already written down the expansion of  $T(k, k, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f)$  in spherical harmonics [see eq. (18.26a)]. We now assert that

$$\delta(\mathbf{k}_f - \mathbf{k}_i) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{1}{\rho(E)} \delta[E(k_i) - E(k_f)] Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) \quad (18.50)$$

with  $E = E(k_i) = E(k_f)$ . Indeed, if we consider a function  $f(\mathbf{k}_i)$  and expand it as

$$f(\mathbf{k}_i) = \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} f_{l'm'}(k_i) Y_{l'm'}(\hat{\mathbf{k}}_i) \quad (18.51)$$

we find by using eq. (18.50) that

$$\begin{aligned} \int \delta(\mathbf{k}_f - \mathbf{k}_i) f(\mathbf{k}_i) d\mathbf{k}_i &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} \int d\Omega_{\mathbf{k}_i} \int_0^{\infty} dk_i k_i^2 \frac{1}{\rho(E)} \\ &\times \delta[E(k_i) - E(k_f)] f_{l'm'}(k_i) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{l'm'}(\hat{\mathbf{k}}_i). \end{aligned} \quad (18.52)$$

Using the orthonormality of the spherical harmonics, we deduce that

$$\begin{aligned} \int \delta(\mathbf{k}_f - \mathbf{k}_i) f(\mathbf{k}_i) d\mathbf{k}_i &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \int_0^{\infty} dk_i k_i^2 \frac{1}{\rho(E)} \delta[E(k_i) - E(k_f)] \\ &\times Y_{lm}(\hat{\mathbf{k}}_f) f_{lm}(k_i). \end{aligned} \quad (18.53)$$

Then, by using eq. (18.24) we obtain

$$\int \delta(\mathbf{k}_f - \mathbf{k}_i) f(\mathbf{k}_i) d\mathbf{k}_i = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \int dE \delta[E(k_i) - E(k_f)] f_{lm}(k_i) Y_{lm}(\hat{\mathbf{k}}_f) \quad (18.54)$$

and therefore

$$\int \delta(\mathbf{k}_f - \mathbf{k}_i) f(\mathbf{k}_i) d\mathbf{k}_i = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} f_{lm}(k_f) Y_{lm}(\hat{\mathbf{k}}_f) = f(\mathbf{k}_f); \quad \text{Q.E.D.} \quad (18.55)$$

We may now use eqs. (18.26a) and (18.50) in eq. (18.49) to obtain the partial wave expansion of the  $S$ -matrix as

$$\begin{aligned} \langle \mathbf{k}_f | S | \mathbf{k}_i \rangle &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{1}{\rho(E)} \delta[E(k_i) - E(k_f)] [1 - 2\pi i \rho(E) T_l(k)] \\ &\times Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) \end{aligned} \quad (18.56)$$

or

$$\langle \mathbf{k}_f | S | \mathbf{k}_i \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{1}{\rho(E)} \delta[E(k_i) - E(k_f)] S_l(k) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) \quad (18.57)$$

with

$$S_l(k) = 1 - 2\pi i \rho(E) T_l(k). \quad (18.58)$$

Using the expression of  $T_l(k)$  given by eq. (18.36), we see that

$$S_l(k) = \exp\{2i\delta_l(k)\}. \quad (18.59)$$

This result agrees with the definition of the “ $S$ -matrix” given in Chapter 4 for the simple case of potential scattering.

It is also convenient to introduce  $S$ -matrix elements  $\langle \hat{\mathbf{k}}_f | S(k) | \hat{\mathbf{k}}_i \rangle$  defined on the *energy-momentum shell* by the relation

$$\langle \hat{\mathbf{k}}_f | S | \hat{\mathbf{k}}_i \rangle = \frac{1}{\rho(E)} \delta[E(k_i) - E(k_f)] \langle \hat{\mathbf{k}}_f | S(k) | \hat{\mathbf{k}}_i \rangle. \quad (18.60)$$

We see from eqs. (18.57)–(18.59) that

$$\langle \hat{\mathbf{k}}_f | S(k) | \hat{\mathbf{k}}_i \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} S_l(k) Y_{lm}(\hat{\mathbf{k}}_f) Y_{lm}^*(\hat{\mathbf{k}}_i) \quad (18.61a)$$

or, by using the addition theorem of spherical harmonics

$$\langle \hat{\mathbf{k}}_f | S(k) | \hat{\mathbf{k}}_i \rangle = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} S_l(k) P_l(\cos \theta) \quad (18.61b)$$

with  $\cos \theta = \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f$ . We note that eq. (18.61a) may be rewritten as

$$\langle \hat{\mathbf{k}}_f | S(k) | \hat{\mathbf{k}}_i \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} \langle \hat{\mathbf{k}}_f | l' m' \rangle \langle l' m' | S(k) | l m \rangle \langle l m | \hat{\mathbf{k}}_i \rangle \quad (18.62)$$

where the spherical harmonics

$$Y_{lm}(\hat{\mathbf{k}}) \equiv \langle \hat{\mathbf{k}} | l m \rangle \quad (18.63)$$

are the transformation functions from the angular momentum representation  $\{l, m\}$  to the plane wave representation  $\{\mathbf{k}\}$ . We also remark that

$$\langle l' m' | S(k) | l m \rangle = \delta_{ll'} \delta_{mm'} S_l(k). \quad (18.64)$$

Hence, in the case of central forces, the  $S$ -matrix is *diagonal in the angular momentum representation*.

Let us now investigate the consequences of the *unitarity condition* on the partial wave scattering matrices. The  $S$  matrix in the angular momentum representation is evidently a diagonal *unitary* matrix with the diagonal elements given by eq. (18.59). To analyze the  $T$  matrix, we start from the operator forms (15.170) of the unitarity relations, namely

$$i(\mathcal{T} - \mathcal{T}^\dagger) = 2\pi \mathcal{T}^\dagger \delta(E - H_0) \mathcal{T} \quad (18.65a)$$

or

$$i(\mathcal{T} - \mathcal{T}^\dagger) = 2\pi \mathcal{T} \delta(E - H_0) \mathcal{T}^\dagger \quad (18.65b)$$

Using eqs. (18.9), we find that

$$\text{Im} T(k_f, k_i, \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f, k) = -\pi \rho(E) \int d\Omega_{\hat{\mathbf{k}}} T^{(+)*}(k, k_f, \hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}_f) T^{(-)}(k, k_i, \hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}_i) \quad (18.66a)$$

and

$$\text{Im} T(k_f, k_i, \hat{k}_i \cdot \hat{k}_f, k) = -\pi \rho(E) \int d\Omega_{\hat{k}} T^{(+)}(k_f, k, \hat{k}' \cdot \hat{k}_f) T^{(-)*}(k_i, k, \hat{k}' \cdot \hat{k}_i) \quad (18.66b)$$

where we have used the fact that  $k' = k$ . On the energy shell ( $k = k_i = k_f$ ), eq. (18.66b) becomes

$$\text{Im} T(k, k, \hat{k}_i \cdot \hat{k}_f) = -\pi \rho(E) \int d\Omega_{\hat{k}} T(k, k, \hat{k}' \cdot \hat{k}_f) T^*(k, k, \hat{k}' \cdot \hat{k}_i). \quad (18.67)$$

We may use eqs. (18.24) and (18.37) to rewrite this relation in terms of the corresponding scattering amplitudes as

$$\text{Im} f(k, \theta) = \frac{k}{4\pi} \int d\Omega_{\hat{k}'} f^*(k, \theta') f(k, \theta_0) \quad (18.68)$$

where  $\cos \theta = \hat{k}_i \cdot \hat{k}_f$ ,  $\cos \theta' = \hat{k}' \cdot \hat{k}_i$  and  $\cos \theta_0 = \hat{k}' \cdot \hat{k}_f$  [6]. This equation is identical to the result (4.94) obtained in Chapter 4.

Let us now analyze these equations in partial waves. From eqs. (18.66) we deduce the off-shell partial wave unitarity relations

$$\text{Im} T_l(k_f, k_i, k) = -\pi \rho(E) T_l^{(+)*}(k, k_f) T_l^{(-)}(k, k_i) \quad (18.69a)$$

and

$$\text{Im} T_l(k_f, k_i, k) = -\pi \rho(E) T_l^{(+)}(k_f, k) T_l^{(-)*}(k_i, k). \quad (18.69b)$$

They reduce on the energy shell to the relation

$$\text{Im} T_l(k) = -\pi \rho(E) |T_l(k)|^2. \quad (18.70)$$

In terms of (on-shell) partial wave amplitudes  $a_l(k) = k^{-1} \exp\{i\delta_l(k)\} \times \sin \delta_l(k)$  such that [see eq. (18.36)]

$$T_l(k) = -\frac{k}{\pi \rho(E)} a_l(k) \quad (18.71)$$

we have therefore

$$\text{Im} a_l(k) = k |a_l(k)|^2 \quad (18.72)$$

which is precisely the result (4.99) obtained for non-relativistic potential scattering of a spinless particle.

Finally, we note that the hermiticity of the  $K$  matrix and the fact that the quantities  $K_l(k)$  are real are also implied by the unitarity condition.

Until now we have expressed the scattering matrices,  $S$ ,  $T$  and  $K$  in the angular momentum representation in terms of phase shifts  $\delta_l^{(S)}(k)$ . To compute these phase shifts we have to analyze the scattering wave functions in partial waves and solve the corresponding radial equations. This was carried out in Chapter 4 for the case of non-relativistic spinless scattering and will

not be repeated here. When the interaction forces are not known, the phase shifts have to be extracted from the experimental data. They play then the role of phenomenological quantities, intermediate between the experimental results and the theoretical expressions obtained for  $S_l$ ,  $T_l$  or  $K_l$ .

To conclude this section we now calculate the cross sections for two-body scattering by central forces. The differential scattering cross section is given by eq. (15.40), namely

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \rho(E) |T_{ba}|^2. \quad (18.73)$$

Using eq. (18.24), together with the fact that  $v_i = dE/(\hbar dk)$ , we find that

$$d\sigma/d\Omega = |f|^2 \quad (18.74)$$

where the scattering amplitude  $f$  is given by eq. (18.39) for the case of spin-independent forces. For spin-dependent (central) forces, we write instead, for a particular value of  $S$ ,

$$d\sigma^{(S)}/d\Omega = |f^{(S)}|^2 \quad (18.75)$$

where  $f^{(S)}$  is given by eq. (18.38). The differential cross section corresponding to a random distribution of initial spin orientations and summed over all final spin orientations is then

$$\frac{d\sigma}{d\Omega} = \frac{1}{(2S_A + 1)(2S_B + 1)} \sum_{S=|S_A-S_B|}^{S_A+S_B} (2S + 1) \frac{d\sigma^{(S)}}{d\Omega}. \quad (18.76)$$

The total cross sections are obtained by integrating the differential cross sections over all scattering angles. For spin-independent forces we find from eqs. (18.42), (18.74), (4.69) and (4.70) that

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l \quad (18.77)$$

in accordance with eq. (4.71). For spin-dependent central forces we may use eqs. (18.43), (18.75), (4.69) and (4.70) to obtain

$$\sigma_{\text{tot}}^{(S)} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l^{(S)}. \quad (18.78)$$

In both cases we may directly verify the *optical theorem* (15.176) by using eqs. (18.42) and (18.43) to calculate  $\text{Im} f(\theta = 0)$  or  $\text{Im} f^{(S)}(\theta = 0)$ . We also note that the total cross section summed over all final spin orientations and averaged over the initial random spin orientations is given by

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \frac{1}{(2S_A + 1)(2S_B + 1)} \sum_{S=|S_A-S_B|}^{S_A+S_B} (2S + 1) \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l^{(S)}. \quad (18.79)$$

## 18.2. Non-central forces. General theory

We now turn to a discussion of the scattering of two particles interacting through non-central forces. Important examples of non-central interactions are the *spin-orbit* and *tensor* forces. The former was first used in atomic physics to describe the interaction of an electron's spin with its orbital angular momentum. It also plays an important role in strong interaction physics. The tensor force was first introduced in connection with the analysis of nucleon-nucleon scattering [7].

As in the case of central forces, it is convenient, especially at low energies, to discuss two-body collisions involving non-central interactions in terms of *phase shifts*. One of the major aims of the theory is therefore to obtain a *generalized partial wave expansion* of the  $S$  matrix. This question will be considered in Section 18.2.1. Another important goal of the theory is to calculate the phase shifts – and thus the amplitudes and cross sections – once the form of the non-central potential is known. We shall discuss this problem in Section 18.2.2. In Section 18.2.3 we introduce the *helicity formalism* [8]. Instead of considering  $S$ -matrix elements between states of total channel spin, orbital angular momentum and total angular momentum, one can use the helicity basis, in which the states are labelled by total angular momenta and projections of the particle spins along their own direction of motion. This approach, as we shall see, has the great advantage that it can be used easily in the relativistic domain and remains valid for massless particles. Finally, in Section 18.2.4, we shall examine the role of *invariance principles* in simplifying the  $S$  matrix. A few important references dealing with the scattering by non-central forces are listed at the end of this chapter [7–19].

### 18.2.1. The generalized partial wave analysis

We begin by examining the problem of finding a generalized partial-wave expansion for the  $S$ -matrix. We consider again two particles A and B, having masses  $m_A$  and  $m_B$ , spins  $S_A$  and  $S_B$ , initial wave vectors  $\mathbf{k}_i$  and  $-\mathbf{k}_i$  and final wave vectors  $\mathbf{k}_f$  and  $-\mathbf{k}_f$  in the C.M. system. The collision leaves the internal states of the particles unaffected, except perhaps for the spin orientations. Conservation of energy therefore implies that  $k_i = k_f$ .

In order to carry out such a partial wave expansion it is useful to introduce new functions  $\mathcal{Y}_{IS}^{JM}$ , associated with the total angular momentum operator  $J$ , and which generalize [20] the spherical harmonics. They are defined by

$$\mathcal{Y}_{IS}^{JM}(\hat{\mathbf{r}}) = \sum_{\substack{m,v \\ (m+v=M)}} \langle ISmv|JM \rangle Y_{lm}(\hat{\mathbf{r}}) \chi_{Sv}. \quad (18.80)$$

The inverse relation

$$Y_{lm}(\hat{\mathbf{r}}) \chi_{Sv} = \sum_{J=|l-S|}^{l+S} \sum_{\mathbf{M}} \langle ISmv|JM \rangle \mathcal{Y}_{IS}^{JM}(\hat{\mathbf{r}}) \quad (18.81)$$

may be obtained by using the orthogonality of the Clebsch–Gordan coefficients, namely [see eq. (E.10) of Appendix E]

$$\sum_{m,v} \langle lSmv | JM \rangle \langle lSmv | J'M' \rangle = \delta_{JJ'} \delta_{MM'}. \quad (18.82)$$

We note that the functions  $\mathcal{Y}_{IS}^{JM}$  are eigenfunctions of the operator  $\mathbf{J}^2$

$$\mathbf{J}^2 \mathcal{Y}_{IS}^{JM} = J(J+1) \hbar^2 \mathcal{Y}_{IS}^{JM} \quad (18.83)$$

of the operator  $\mathbf{J}_z$ ,

$$\mathbf{J}_z \mathcal{Y}_{IS}^{JM} = M \hbar \mathcal{Y}_{IS}^{JM} \quad (18.84)$$

of  $L^2$ ,

$$\mathbf{L}^2 \mathcal{Y}_{IS}^{JM} = l(l+1) \hbar^2 \mathcal{Y}_{IS}^{JM} \quad (18.85)$$

and of  $S^2$ ,

$$\mathbf{S}^2 \mathcal{Y}_{IS}^{JM} = S(S+1) \hbar^2 \mathcal{Y}_{IS}^{JM}. \quad (18.86)$$

Furthermore, if  $\mathcal{P}$  is the parity operator defined by eqs. (16.186), we also have

$$\mathcal{P} \mathcal{Y}_{IS}^{JM} = (-)^l \mathcal{Y}_{IS}^{JM}. \quad (18.87)$$

As we have already noted in dealing with central forces, two particular bases in spin space are usually employed to represent the spin states of the system of two particles. The first one, or  $\{\nu_A, \nu_B\}$  representation, is the natural basis to discuss polarization phenomena (see Section 18.3.3). On the other hand, the  $\{S, \nu\}$  representation, which is more convenient to carry out the phase shift analysis, will be used here. We first add the spins of the two colliding particles to obtain a total spin  $S$  with component  $\nu$  along the axis of quantization. The initial free wave is then given in the coordinate representation by

$$\langle \mathbf{r} | \Phi_a \rangle \equiv \langle \mathbf{r} | \mathbf{k}_i, S, \nu \rangle \equiv \Phi_{\mathbf{k}_i, S, \nu}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \chi_{S\nu} \quad (18.88)$$

where  $\chi_{S\nu}$  is given by eq. (18.14). The corresponding free final state is

$$\langle \mathbf{r} | \Phi_b \rangle \equiv \langle \mathbf{r} | \mathbf{k}_f, S', \nu' \rangle \equiv \Phi_{\mathbf{k}_f, S', \nu'}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}) \chi_{S'\nu'}. \quad (18.89)$$

and these free states are normalized in such a way that

$$\langle \mathbf{k}_f, S', \nu' | \mathbf{k}_i, S, \nu \rangle = \delta(\mathbf{k}_i - \mathbf{k}_f) \delta_{SS'} \delta_{\nu\nu'}. \quad (18.90)$$

Let us introduce the auxiliary functions

$$Z_{IS\nu}^{JM}(\hat{\mathbf{k}}) = \sum_{m=-l}^{+l} \langle lSmv | JM \rangle Y_{lm}(\hat{\mathbf{k}}). \quad (18.91)$$

We may then decompose the initial free wave as

$$\Phi_{\mathbf{k}_i, S, \nu} = (2/\pi)^{1/2} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(k_i r) Y_{lm}^*(\hat{\mathbf{k}}_i) Y_{lm}(\hat{\mathbf{r}}) \chi_{S\nu} \quad (18.92)$$



or

$$\Phi_{k_i, S, v} = (2/\pi)^{1/2} \sum_{J=|S|}^{J+S} \sum_M i^J j_l(k_i r) Z_{lSv}^{JM*}(\hat{k}_i) \mathcal{Y}_{lS}^{JM}(\hat{r}) \quad (18.93)$$

where we have used eqs. (18.80) and (18.91). We may also define the quantities [21]

$$\langle \hat{l}' S' v' | \mathcal{Y}^J | \hat{k}_i l S v \rangle = \sum_{m', m, M} Y_{l'm'}(\hat{r}) Y_{lm}^*(\hat{k}_i) \langle l' S' m' v' | JM \rangle \langle l S m v | JM \rangle \quad (18.94)$$

to write

$$\Phi_{k_i, S, v} = (2/\pi)^{1/2} \sum_{l, J} i^J j_l(k_i r) \langle \hat{l}' l S v | \mathcal{Y}^J | \hat{k}_i l S v \rangle \chi_{Sv}. \quad (18.95)$$

Since we assume that the Hamiltonian is invariant under rotations, we want to decompose the  $S$  matrix into submatrices corresponding to states of definite total angular momentum  $J$ . To this end, we first introduce the  $S$ -matrix elements on the energy-momentum shell  $\langle \hat{k}_f, S', v' | S(k) | \hat{k}_i, S, v \rangle$  by the relations [cf. eq. (18.60)]

$$\langle \hat{k}_f, S', v' | S(k) | \hat{k}_i, S, v \rangle = \frac{1}{\rho(E)} \delta[E(k_i) - E(k_f)] \langle \hat{k}_f, S', v' | S(k) | \hat{k}_i, S, v \rangle, \quad (18.96)$$

where  $k = k_i = k_f$ . We then write, as in eq. (18.62)

$$\begin{aligned} \langle \hat{k}_f, S', v' | S(k) | \hat{k}_i, S, v \rangle &= \sum_l \sum_m \sum_{l'} \sum_{m'} \langle \hat{k}_f S' v' | l' m' S' v' \rangle \\ &\times \langle l' m' S' v' | S(k) | l m S v \rangle \langle l m S v | \hat{k}_i S v \rangle. \end{aligned} \quad (18.97)$$

Next, we remember that

$$Y_{lm}(\hat{k}) = \langle \hat{k} S v | l m S v \rangle$$

and we express the states  $|l' m' S' v'\rangle$  and  $|l m S v\rangle$  (and the corresponding bras) in the  $\{l', S', J', M'\}$  and  $\{l, S, J, M\}$  representations, using Clebsch-Gordan coefficients. Then eq. (18.97) becomes

$$\begin{aligned} \langle \hat{k}_f, S', v' | S(k) | \hat{k}_i, S, v \rangle &= \sum_{l m l' m'} \sum_{J M J' M'} Y_{l' m'}(\hat{k}_f) \\ &\times \langle l' S' m' v' | JM \rangle \langle l' S' J' M' | S(k) | l S J M \rangle \langle l S m v | JM \rangle Y_{lm}^*(\hat{k}_i). \end{aligned}$$

We may now invoke the rotational invariance of  $H$  to deduce from eq. (16.184) that the  $S$  matrix is diagonal in  $J$  and  $M$  and independent of  $M$ . Thus we have

$$\langle l' S' J' M' | S(k) | l S J M \rangle = \delta_{JJ'} \delta_{MM'} \langle l' S' | S^J(k) | l S \rangle \quad (18.98)$$

and using the definition (18.94), we obtain

$$\langle \hat{k}_f, S', v' | S(k) | \hat{k}_i, S, v \rangle = \sum_{l l'} \langle \hat{k}_f l' S' v' | \mathcal{Y}^J | \hat{k}_i l S v \rangle \langle l' S' | S^J(k) | l S \rangle. \quad (18.99)$$

This is the generalized partial wave expansion of the  $S$  matrix. We note that the  $S$ -matrix elements (18.98) do not require that  $l = l'$ ,  $S = S'$ , since the spin and orbital angular momentum are not necessarily conserved [22].

A similar decomposition may be written down for the  $T$ -matrix elements. We first write the  $S$ -matrix element in the C.M. sub-space (on the momentum shell) as

$$\begin{aligned} \langle \mathbf{k}_f, S', v' | S | \mathbf{k}_i, S, v \rangle &= \delta(\mathbf{k}_i - \mathbf{k}_f) \delta_{SS'} \delta_{vv'} \\ &\quad - 2\pi i \delta[E(k_i) - E(k_f)] \langle \mathbf{k}_f, S', v' | T(k) | \mathbf{k}_i, S, v \rangle \end{aligned} \quad (18.100)$$

where

$$\langle \mathbf{k}_f, S', v' | T(k) | \mathbf{k}_i, S, v \rangle \equiv [\langle \mathbf{k}_f, S', v' | T | \mathbf{k}_i, S, v \rangle]_{k_i = k_f = k}$$

is the  $T$ -matrix element on the energy shell. We now resolve these  $T$ -matrix elements as

$$\langle \mathbf{k}_f, S', v' | T(k) | \mathbf{k}_i, S, v \rangle = \sum_{l'l''} \langle \mathbf{k}_f l' S' v' | \mathcal{Q}^J | \mathbf{k}_i l S v \rangle \langle l' S' | T^J(k) | l S \rangle \quad (18.101)$$

which is a generalization of eq. (18.26a). Similar decompositions also hold for the off-the-energy shell  $T$ -matrix elements and for the  $K$ -matrix elements. Using the above relations we then have

$$\langle l' S' | S^J(k) | l S \rangle = \delta_{ll'} \delta_{SS'} - 2\pi i \rho(E) \langle l' S' | T^J(k) | l S \rangle. \quad (18.102)$$

The differential cross section corresponding to a process  $\mathbf{k}_i, S, v \rightarrow \mathbf{k}_f, S', v'$  is given by eq. (15.40) which we write explicitly as

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \rho(E) |\langle \mathbf{k}_f, S', v' | T(k) | \mathbf{k}_i, S, v \rangle|^2. \quad (18.103)$$

For unpolarized beams and targets, this cross section must be summed over  $S$  and  $v$  and divided by the total number  $(2S_A + 1)(2S_B + 1)$  of initial spin orientations. Furthermore, if all the final states  $(S', v')$  are recorded without discrimination by the counting apparatus, we must also sum over all  $S', v'$ . The resulting average cross section is then

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{(2S_A + 1)(2S_B + 1)} \sum_{S, v, S', v'} \frac{d\sigma}{d\Omega} \quad (18.104)$$

where  $d\sigma/d\Omega$  is given by eq. (18.103).

### 18.2.2. The radial equations

Let us now return to the Lippmann-Schwinger equation (16.3) with  $V_i = V_f = V$ . In the position representation  $\{\mathbf{r}\}$  we may write

$$\langle \mathbf{r} | \Psi_a^{(+)} \rangle \equiv \Psi_{\mathbf{k}_i, S, v}^{(+)}(\mathbf{r}) = \Phi_{\mathbf{k}_i, S, v}(\mathbf{r}) + \int \mathcal{G}_0^{(+)}(k_i, \mathbf{r}, \mathbf{r}') V(\mathbf{r}') \Psi_{\mathbf{k}_i, S, v}^{(+)}(\mathbf{r}') d\mathbf{r}' \quad (18.105)$$

where the interaction operator  $V$  is now in general spin-dependent and the Green's function  $\mathcal{G}_0^{(+)}(k_i, \mathbf{r}, \mathbf{r}')$  is given by

$$\mathcal{G}_0^{(+)}(k_i, \mathbf{r}, \mathbf{r}') = \sum_{S', v'} \int d\mathbf{k}' \frac{\Phi_{\mathbf{k}', S', v'}(\mathbf{r}) \Phi_{\mathbf{k}', S', v'}^{\dagger}(\mathbf{r}')}{E_a(k_i) - E(k') + i\epsilon}. \quad (18.106)$$

Here we have used the completeness of the free states, namely

$$\sum_{S', v'} \int d\mathbf{k}' |\mathbf{k}' S' v'\rangle \langle \mathbf{k}' S' v'| = 1. \quad (18.107a)$$

We note that in the position representation

$$\begin{aligned} & \sum_{S', v'} \int d\mathbf{k}' \Phi_{\mathbf{k}' S' v'}(\mathbf{r}) \Phi_{\mathbf{k}' S' v'}^\dagger(\mathbf{r}) \\ &= (2\pi)^{-3} \sum_{S', v'} \int d\mathbf{k}' \exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\} \chi_{S' v'} \chi_{S' v'}^\dagger = \delta(\mathbf{r} - \mathbf{r}') \end{aligned} \quad (18.107b)$$

where we have used the fact that

$$\sum_{S', v'} \chi_{S' v'} \chi_{S' v'}^\dagger = 1. \quad (18.107c)$$

Returning to eq. (18.110), we see that

$$\mathcal{G}_0^{(+)}(k_i, \mathbf{r}, \mathbf{r}') = -(2\pi)^{-3} \sum_{S', v'} \int d\mathbf{k}' \frac{\exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\}}{E(k') - E_a(k_i) - i\varepsilon} \chi_{S' v'} \chi_{S' v'}^\dagger \quad (18.108a)$$

$$= -(2\pi)^{-3} \int d\mathbf{k}' \frac{\exp\{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\}}{E(k') - E_a(k_i) - i\varepsilon}. \quad (18.108b)$$

Let us first analyze the behaviour of the Lippmann-Schwinger equation (18.105) when  $r \rightarrow \infty$ . To this end, we first note that for any bounded function  $F(\mathbf{k}_i, \mathbf{k}')$  we have

$$\lim_{r \rightarrow \infty} \int d\mathbf{k}' \frac{\exp(i\mathbf{k}' \cdot \mathbf{r})}{E(k') - E_a(k_i) - i\varepsilon} F(\mathbf{k}_i, \mathbf{k}') = (2\pi)^2 k_i \frac{d k_i}{d E_a} \frac{e^{i k_i r}}{r} F(\mathbf{k}_i, \mathbf{k}_f) \quad (18.109)$$

with  $\mathbf{k}_f = k_i \hat{\mathbf{r}}$ . Thus we may write

$$\begin{aligned} \Psi_{\mathbf{k}_i, S, v}^{(+)}(\mathbf{r}) &\xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left\{ \exp\{i\mathbf{k}_i \cdot \mathbf{r}\} \chi_{S, v} \right. \\ &\quad \left. + \frac{e^{i k_i r}}{r} \sum_{S', v'} \left[ -(2\pi)^2 k \frac{d k}{d E} \langle \hat{\mathbf{k}}_f, S', v' | T(k) | \hat{\mathbf{k}}_i, S, v \rangle \right] \chi_{S', v'} \right\} \end{aligned} \quad (18.110)$$

where we have set  $k = |\mathbf{k}_i| = |\mathbf{k}_f|$  and the on-shell reduced  $T$ -matrix element appearing in this equation is given by

$$\langle \hat{\mathbf{k}}_f, S', v' | T(k) | \hat{\mathbf{k}}_i, S, v \rangle = [\langle \Phi_{\mathbf{k}_i, S', v'} | V | \Psi_{\mathbf{k}_i, S, v}^{(+)} \rangle]_{k_i = k_f = k}. \quad (18.111)$$

It is convenient at this point to introduce a generalized scattering amplitude operator  $M(\mathbf{k}_f, \mathbf{k}_i, S_A, S_B)$  such that, in the  $\{S, v\}$  representation, the corresponding  $(2S_A + 1)(2S_B + 1) \times (2S_A + 1)(2S_B + 1)$  matrix in spin space is given by

$$\begin{aligned} \langle S', v' | M | S, v \rangle &= \langle \chi_{S' v'} | M(\mathbf{k}_f, \mathbf{k}_i, S_A, S_B) | \chi_{S v} \rangle \\ &= -(2\pi)^2 k \frac{d k}{d E} \langle \hat{\mathbf{k}}_f, S', v' | T(k) | \hat{\mathbf{k}}_i, S, v \rangle. \end{aligned} \quad (18.112)$$

In the  $\{v_A, v_B\}$  representation the same operator is represented by the  $(2S_A + 1)(2S_B + 1) \times (2S_A + 1)(2S_B + 1)$  matrix

$$\begin{aligned} \langle v'_A, v'_B | M | v_A, v_B \rangle &= \langle \chi_{S_A v'_A} \chi_{S_B v'_B} | M(\mathbf{k}_f, \mathbf{k}_i, S_A, S_B) | \chi_{S_A v_A} \chi_{S_B v_B} \rangle \\ &= -(2\pi)^2 k \frac{dk}{dE} \langle \hat{\mathbf{k}}_f, v'_A, v'_B | T(k) | \hat{\mathbf{k}}_i, v_A, v_B \rangle. \end{aligned} \quad (18.113)$$

Using eq. (18.101) we may also write eq. (18.112) as

$$\langle S', v' | M | S, v \rangle = 4\pi \sum_{l, l', J} \langle \hat{\mathbf{k}}_f l' S' v' | \mathcal{Y}^J | \hat{\mathbf{k}}_i l S v \rangle \langle l' S' | a^J(k) | l S \rangle \quad (18.114)$$

with [compare with eq. (4.65)]

$$\begin{aligned} \langle l' S' | a^J(k) | l S \rangle &= -\pi k \frac{dk}{dE} \langle l' S' | T^J(k) | l S \rangle \\ &= \frac{1}{2ik} [\langle l' S' | S^J(k) | l S \rangle - \delta_{ll'} \delta_{SS'}]. \end{aligned} \quad (18.115)$$

Returning to eq. (18.110), we may write with the help of eq. (18.112)

$$\Psi_{\mathbf{k}_i, S, v}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) \chi_{Sv} + \frac{e^{ikr}}{r} \sum_{S', v'} \langle S', v' | M | S, v \rangle \chi_{S' v'} \right] \quad (18.116)$$

while, from eqs. (18.103) and (18.112) we deduce that the differential cross section for the transition  $(\mathbf{k}_i, S, v) \rightarrow (\mathbf{k}_f, S', v')$  is given by

$$\frac{d\sigma}{d\Omega} = |\langle S', v' | M | S, v \rangle|^2. \quad (18.117)$$

The generalized partial wave analysis of the Lippmann-Schwinger equation (18.105) may be carried out as in the simple cases of potential scattering (see Section 5.4) or two-body scattering with central forces. We shall only consider here non-relativistic collisions, so that

$$E_a(k_i) = \hbar^2 k^2 / 2m$$

where we have set  $k_i = k$  and

$$m = m_A m_B / (m_A + m_B). \quad (18.118)$$

We first expand

$$\Psi_{\mathbf{k}_i, S, v}^{(+)}(\mathbf{r}) = \sum_{l' S' l J M} R_{l' S', l S}^J(k, r) Z_{l S v}^{J M*}(\hat{\mathbf{k}}) \mathcal{Y}_{l' S'}^{J M}(\hat{\mathbf{r}}) \quad (18.119a)$$

$$= (2/\pi)^{1/2} \sum_{l' S' v' l J} i^{l'} \langle \hat{\mathbf{r}} l' S' v' | \mathcal{Y}^J | \hat{\mathbf{k}}_i l S v \rangle R_{l' S', l S}^J(k, r) \chi_{S' v'} \quad (18.119b)$$

where  $R_{l' S', l S}^J(k, r)$  are the radial functions which generalize [23] the functions  $R_l(k, r)$  introduced in Chapter 4. Furthermore we may use eq. (5.89) to write the Green's function (18.108b) as

$$\begin{aligned} \mathcal{G}_0^{(+)}(k, \mathbf{r}, \mathbf{r}') &= \frac{2m}{\hbar^2} \left( -\frac{1}{4\pi} \frac{\exp\{ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \right) \\ &= \frac{2m}{\hbar^2} \sum_{l, m} g_l^{(+)}(k, r, r') Y_{lm}^*(\hat{\mathbf{r}}') Y_{lm}(\hat{\mathbf{r}}) \\ &= \frac{2m}{\hbar^2} \sum_{J M l S} g_l^{(+)}(k, r, r') \mathcal{Y}_{l S}^{J M*}(\hat{\mathbf{r}}') \mathcal{Y}_{l S}^{J M}(\hat{\mathbf{r}}) \end{aligned} \quad (18.120a)$$

with

$$g_l^{(+)}(k, r, r') = -ikj_l(kr_<)h_l^{(1)}(kr_>). \quad (18.120b)$$

We now insert the expansions (18.93), (18.119) and (18.120) in the Lippmann–Schwinger equation (18.105) to obtain the set of *coupled* integral equations [compare with eq. (5.98)]

$$R_{l'S',lS}^J(k, r) = j_l(kr)\delta_{ll'}\delta_{SS'} + \sum_{l''S''} \int_0^\infty dr' r'^2 g_l^{(+)}(k, r, r') \mathcal{V}_{l'S',l''S''}^J(r') R_{l''S'',lS}^J(k, r') \quad (18.121)$$

where

$$\mathcal{V}_{l'S',l''S''}^J(r) = \frac{2m}{\hbar^2} \int d\Omega_{\hat{r}} \mathcal{Y}_{l'S'}^{JM*}(\hat{r}) V(r) \mathcal{Y}_{l''S''}^{JM}(\hat{r}) \quad (18.122)$$

is the (reduced) *potential matrix*. We have adopted for the scattering wave functions the “normalization” [see eq. (18.90)]

$$\langle \Psi_{k',S',v'}^{(+)} | \Psi_{k,S,v}^{(+)} \rangle = \delta(k' - k) \delta_{SS'} \delta_{vv'} \quad (18.123)$$

so that, from eqs. (18.119), we have

$$\sum_{l''S''} \int_0^\infty dr r^2 [R_{l''S'',l'S}^J(k', r)]^* R_{l''S'',lS}^J(k, r) = \frac{\pi}{2k^2} \delta(k - k') \delta_{ll'} \delta_{SS'}. \quad (18.124)$$

To investigate the behaviour of the radial wave functions at large  $r$  we use the fact that [see eqs. (18.120b) and (C.12c) of Appendix C]

$$g_l^{(+)}(k, r, r') \xrightarrow{r \rightarrow \infty} -\frac{e^{ikr}}{r} (-i)^l j_l(kr'). \quad (18.125)$$

Hence we see from eq. (18.121) that

$$R_{l'S',lS}^J(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) \delta_{ll'} \delta_{SS'} - \frac{e^{ikr}}{r} (-i)^{l'} \sum_{l''S''} \int_0^\infty dr' r'^2 j_l(kr') \times \mathcal{V}_{l'S',l''S''}^J(r') R_{l''S'',lS}^J(k, r'). \quad (18.126a)$$

Alternatively, we may also use eqs. (18.95) and (18.101) to infer from eq. (18.110) that

$$R_{l'S',lS}^J(k, r) \xrightarrow{r \rightarrow \infty} j_l(kr) \delta_{ll'} \delta_{SS'} - \frac{e^{ikr}}{r} (-i)^{l'} \pi k \frac{dk}{dE} \langle l'S' | T^J(k) | lS \rangle \quad (18.126b)$$

and therefore

$$\langle l'S' | T^J(k) | lS \rangle = (\pi k)^{-1} \frac{dE}{dk} \sum_{l''S''} \int_0^\infty dr r^2 j_l(kr) \mathcal{V}_{l'S',l''S''}^J(r) R_{l''S'',lS}^J(k, r). \quad (18.127)$$

From eq. (18.102) we also have [with  $\rho(E) = k^2 dk/dE$ ]

$$\begin{aligned} \langle l'S'|S^J(k)|lS\rangle &= \delta_{ll'}\delta_{SS'} - 2ik \sum_{l''S''} \int_0^\infty dr r^2 j_l(kr) \\ &\quad \times \mathcal{V}_{l'S',l''S''}^J(r) R_{l''S'',lS}^J(k, r). \end{aligned} \quad (18.128)$$

Finally, by using the asymptotic behaviour of the spherical Bessel function  $j_l(kr)$  [see eq. (C.12a) of Appendix C] we have

$$R_{l'S',lS}^J(k, r) \xrightarrow{r \rightarrow \infty} \frac{i^{-(l'+1)}}{2kr} \{ -(-1)^l \delta_{ll'} \delta_{SS'} e^{-ikr} + \langle l'S'|S^J(k)|lS\rangle e^{ikr} \}. \quad (18.129)$$

As in Chapter 4 it is also convenient to introduce the new radial functions

$$u_{l'S',lS}^J(k, r) = A_{l'}(k) r R_{l'S',lS}^J(k, r) \quad (18.130)$$

where the coefficients  $A_{l'}(k)$  are fixed by the “normalization” which we impose on  $u_{l'S',lS}^J$ . We then have [compare with eq. (4.48)]

$$u_{l'S',lS}^J(k, r) \xrightarrow{r \rightarrow \infty} \tilde{A}_{l'}(k) \{ \langle l'S'|S^J(k)|lS\rangle e^{ikr} - (-1)^l \delta_{ll'} \delta_{SS'} e^{-ikr} \} \quad (18.131)$$

where

$$\tilde{A}_{l'}(k) = i^{-(l'+1)} A_{l'}(k)/2k. \quad (18.132)$$

Starting from the radial integral equations (18.121), it is a simple matter to verify that the new radial functions  $u_{l'S',lS}^J$  satisfy the *coupled* Schrödinger equations

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l'(l'+1)}{r^2} \right] u_{l'S',lS}^J(k, r) = \sum_{l''S''} \mathcal{V}_{l'S',l''S''}^J(r) u_{l''S'',lS}^J(k, r). \quad (18.133)$$

It is worth noting that the functions  $u_{l'S',lS}^J$  are in general complex. Moreover, the coupled equations (18.133) have different centrifugal terms and therefore the solutions have a different behaviour at the origin. Apart from these (minor) complications, the solutions of the coupled equations proceeds as in the case of central forces [24]. Most of the discussion of Chapter 11 concerning the analytic properties of scattering amplitudes may also be generalized to the case of two-body scattering by non-central forces [25, 26].

Before we proceed to examine the helicity formalism, it is important to note that our discussion of two-body scattering may easily be generalized to the case of two-body *reactions* of the type

$$A + B \rightarrow C + D$$

where the particles A, B, C and D may be *composite*. In this case, of course, the term “two-body” only refers to the fact that there are two particles in the initial and final states, even though several “elementary” particles may be involved in the collision. The initial free state is then described in the

coordinate representation by

$$\langle \mathbf{r}_i, \xi_i | i, \mathbf{k}_i, n, S, v \rangle \equiv \Phi_{i, \mathbf{k}_i, n, S, v}(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_i) \varphi_{i, n, S, v}(\xi_i) \quad (18.134)$$

where the subscript  $i$  refers to the initial arrangement channel  $i$ , the index  $n$  summarizes all the internal quantum numbers of the initial channel (except  $S$  and  $v$ ) and  $\xi_i$  represents symbolically the set of internal coordinates of the particles in channel  $i$ . Here we work in the  $\{S, v\}$  representation, having combined the spins  $S_A$  and  $S_B$  to obtain the resultant spin  $S$  with azimuthal component  $v$ . We have denoted by  $\varphi_{i, n, S, v}(\xi_i)$  the corresponding eigenstate of the internal Hamiltonian  $h_i$  of channel  $i$  [see eq. (14.130)]. We shall also denote the initial energy by  $E_i(k_i)$  and the corresponding density of states by  $\rho_i = k_i^2 dk_i/dE_i$ . In the final state we have  $E_f(k_f)$ ,  $\rho_f = k_f^2 dk_f/dE_f$  and

$$\langle \mathbf{r}_f, \xi_f | f, \mathbf{k}_f, n', S', v' \rangle \equiv \Phi_{f, \mathbf{k}_f, n', S', v'} = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_f) \varphi_{f, n', S', v'}(\xi_f). \quad (18.135)$$

Defining now the  $S$ -matrix elements on the energy-momentum shell by [27]

$$\begin{aligned} \langle f, \mathbf{k}_f, n', S', v' | S | i, \mathbf{k}_i, n, S, v \rangle &= [\rho_i \rho_f]^{-1/2} \delta[E_i(k_i) - E_f(k_f)] \\ &\times \langle f, \hat{\mathbf{k}}_f, n', S', v' | S(k_i) | i, \hat{\mathbf{k}}_i, n, S, v \rangle \end{aligned} \quad (18.136)$$

we may generalize eq. (18.99) to read

$$\begin{aligned} \langle f, \hat{\mathbf{k}}_f, n', S', v' | S(k_i) | i, \hat{\mathbf{k}}_i, n, S, v \rangle &= \sum_{ll'J} \langle \hat{\mathbf{k}}_f l' S' v' | \mathcal{Q}^J | \hat{\mathbf{k}}_i l S v \rangle \\ &\times \langle f n' l' S' | S^J(k_i) | i n l S \rangle. \end{aligned} \quad (18.137)$$

We also have

$$\begin{aligned} \langle f, \mathbf{k}_f, n', S', v' | S | i, \mathbf{k}_i, n, S, v \rangle &= \delta_{fi} \delta_{n'n} \delta_{S'S} \delta_{v'v} \delta(\mathbf{k}_i - \mathbf{k}_f) \\ &- 2\pi i \delta(E_i - E_f) \langle f, \hat{\mathbf{k}}_f, n', S', v' | T(k_i) | i, \hat{\mathbf{k}}_i, n, S, v \rangle \end{aligned} \quad (18.138)$$

with

$$\langle f, \hat{\mathbf{k}}_f, n', S', v' | T(k_i) | i, \hat{\mathbf{k}}_i, n, S, v \rangle \equiv [\langle f, \mathbf{k}_f, n', S', v' | T | i, \mathbf{k}_i, n, S, v \rangle]_{E_i=E_f}. \quad (18.139)$$

We may also decompose the  $T$ -matrix elements (on the energy shell) as

$$\begin{aligned} \langle f, \hat{\mathbf{k}}_f, n', S', v' | T(k_i) | i, \hat{\mathbf{k}}_i, n, S, v \rangle &= \sum_{ll'J} \langle \hat{\mathbf{k}}_f l' S' v' | \mathcal{Q}^J | \hat{\mathbf{k}}_i l S v \rangle \\ &\times \langle f n' l' S' | T^J(k_i) | i n l S \rangle. \end{aligned} \quad (18.140)$$

As a generalization of eq. (18.102) we have

$$\langle f n' l' S' | S^J(k_i) | i n l S \rangle = \delta_{fi} \delta_{nn'} \delta_{SS'} - 2\pi i [\rho_i \rho_f]^{1/2} \langle f n' l' S' | T^J(k_i) | i n l S \rangle \quad (18.141)$$

while eq. (18.103) now becomes

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \rho_f |\langle f, \hat{\mathbf{k}}_f, n', S', v' | T(k_i) | i, \hat{\mathbf{k}}_i, n, S, v \rangle|^2. \quad (18.142)$$

### 18.2.3. The helicity formalism

We have thus far coupled the initial spins  $S_A$  and  $S_B$  to form a resultant spin  $S$  with projection  $v$  along a fixed quantization axis. This resultant spin was then coupled to the relative orbital angular momentum; the same operation was done in the final state. An element of  $S^J(k)$  was then called [28]  $\langle l'S'|S^J(k)|lS\rangle$ . It is also worth noting that we used a fixed axis of spin quantization. This simplifies the description of the initial state but leads to difficulties in handling the final state. The formulae thus obtained, involving Clebsch–Gordan coefficients, are complicated. Another drawback of the separation of the total angular momentum operator into a relative orbital and a spin part is that it leads to complications in the relativistic case and breaks down in particular for massless particles. Finally, the introduction of the total spin  $S$  leads to complicated formulae when dealing with polarization phenomena.

We shall now briefly [29] describe an alternative way of analyzing two-body collisions involving particles with spin. The crucial point is to note that the projection  $\lambda$  of the spin  $s$  of a particle (having momentum  $p$  and energy  $E$ ) along its direction of motion  $\hat{p}$  is invariant under rotations. Indeed, this projection  $\lambda$ , which is called the *helicity quantum number* or simply the *helicity*, may also be considered as the projection of the *total* angular momentum  $J$  along the direction of motion (since the orbital angular momentum has no component along  $\hat{p}$ ), and we know that the projection of  $J$  along a given axis – which is chosen here to be the direction of motion – is invariant under rotations.

Since the helicity  $\lambda$  is invariant under rotations, it is possible to construct *helicity states* having specified values of the quantum numbers  $J$  and  $M$ , and in which all the particles involved have definite helicities. For a two-body collision  $A + B \rightarrow C + D$  in the C.M. system we may then write the  $S$ -matrix element for a transition  $(k_i, J, M, \lambda_A, \lambda_B) \rightarrow (k_f, J', M', \lambda_C, \lambda_D)$  as

$$\begin{aligned} \langle k_f, J', M', \lambda_C, \lambda_D | S | k_i, J, M, \lambda_A, \lambda_B \rangle \\ = \delta[E_f(k_f) - E_i(k_i)] \delta_{JJ'} \delta_{MM'} \langle \lambda_C, \lambda_D | S^J(k_i) | \lambda_A, \lambda_B \rangle \end{aligned} \quad (18.143)$$

where  $\lambda_A, \lambda_B, \lambda_C$  and  $\lambda_D$  denote respectively the helicities of the particles A, B, C and D.

Before we study in more detail the helicity states, let us state some important facts [8, 30] concerning the plane-wave solutions of the wave equations for particles of mass  $m$ , spin  $s$ , momentum  $p$  and energy  $E = c(m^2c^2 + p^2)^{1/2}$ .

i) For each  $p$ , and with  $m \neq 0$ , there are  $2s + 1$  linearly independent solutions which may be chosen to be states of definite helicity:

$$\lambda = s, s - 1, \dots, -s + 1, -s. \quad (18.144)$$

If  $m = 0$ , there are only two solutions, corresponding to

$$\lambda = \pm s. \quad (18.145)$$



ii) When a rotation is applied to one of these solutions, one obtains a state with a different direction of  $\mathbf{p}$ , but the same helicity  $\lambda$ .

iii) When a space reflection is applied, the helicity  $\lambda$  changes sign.

iv) If a Lorentz transformation parallel to  $\mathbf{p}$  is applied, one obtains a state with the same (or the opposite) direction of  $\mathbf{p}$ , but a different magnitude of  $\mathbf{p}$ . If the direction of  $\mathbf{p}$  is *not* reversed,  $\lambda$  remains unchanged.

Let us first agree on a convention to specify the relative phases of these basic free-particle states. This may be done in the following way. Firstly, according to the statement ii) made above the states with momentum  $\mathbf{p}'$  in a direction given by the polar angles  $(\theta, \phi)$  may be defined by applying to the states  $\psi_{\mathbf{p},\lambda}$  having momentum  $\mathbf{p}$  in the positive  $z$  direction and helicity  $\lambda$  a *rotation* through an angle  $\theta$  in the positive sense about the axis  $\mathbf{p} \times \mathbf{p}'$ . (The positive sense of rotation is defined from  $\mathbf{p}$  toward  $\mathbf{p}'$  as a right-hand screw.) We shall now show that such a rotation may be written as

$$|p\theta\phi, \lambda\rangle = R_{\phi,\theta,-\phi}\psi_{\mathbf{p},\lambda} \quad (18.146)$$

where

$$R_{\alpha\beta\gamma} = \exp(-i\alpha J_z) \exp(-i\beta J_y) \exp(-i\gamma J_z) \quad (18.147)$$

is the rotation operator corresponding to the three Euler angles,  $\alpha, \beta, \gamma$  (with  $\hbar = 1$ ) and  $J_x, J_y, J_z$  are the projections of the total angular momentum operator  $\mathbf{J}$  of the particle along the coordinate axes. As shown in Fig. 18.1, the three Euler angles are defined by the following successive rotations

- (1) a rotation about the  $z$ -axis, of angle  $\alpha$ ,
- (2) a rotation about the  $y'$ -axis, of angle  $\beta$ ,
- (3) a rotation about the  $Z$ -axis, of angle  $\gamma$ .

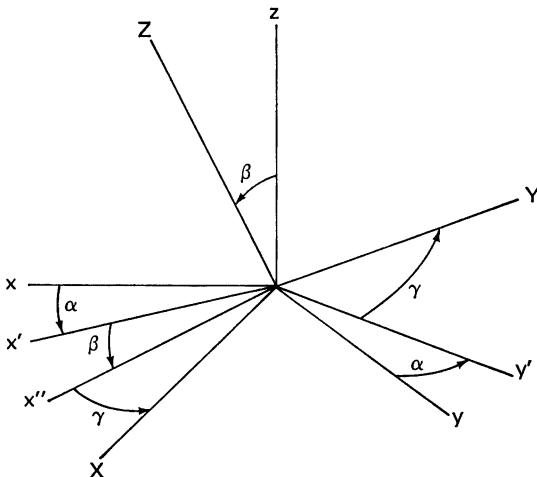


Fig. 18.1. The Euler angles  $\alpha, \beta, \gamma$  of the text.

We note that  $0 \leq \alpha < 2\pi$ ,  $0 \leq \beta \leq \pi$  and  $0 \leq \gamma \leq 2\pi$ . The unitary operators  $\exp(-i\alpha J_z)$ ,  $\exp(-i\beta J_{y'})$  and  $\exp(-i\gamma J_z)$  correspond respectively to a rotation of  $\alpha$  about the  $z$  axis, of  $\beta$  about the  $y'$  axis and of  $\gamma$  about the  $Z$  axis. A general rotation, corresponding to the three Euler angles  $\alpha$ ,  $\beta$ ,  $\gamma$  is therefore specified by the rotation operator

$$R_{\alpha\beta\gamma} = \exp(-i\gamma J_z) \exp(-i\beta J_{y'}) \exp(-i\alpha J_z). \quad (18.148)$$

To show the equivalence of eqs. (18.147) and (18.148), we first note that

$$J_{y'} = \exp(-i\alpha J_z) J_y \exp(i\alpha J_z) \quad (18.149)$$

so that

$$\exp(-i\beta J_{y'}) = \exp(-i\alpha J_z) \exp(-i\beta J_y) \exp(i\alpha J_z) \quad (18.150)$$

and

$$\begin{aligned} J_z &= \exp(-i\beta J_{y'}) J_z \exp(i\beta J_{y'}) \\ &= \exp(-i\alpha J_z) \exp(-i\beta J_y) J_z \exp(i\beta J_y) \exp(i\alpha J_z) \end{aligned}$$

which implies that

$$\exp(-i\gamma J_z) = \exp(-i\alpha J_z) \exp(-i\beta J_y) \exp(-i\gamma J_z) \exp(i\beta J_y) \exp(i\alpha J_z). \quad (18.151)$$

Upon substitution of eqs. (18.150) and (18.151) in eq. (18.148) we find the result (18.147).

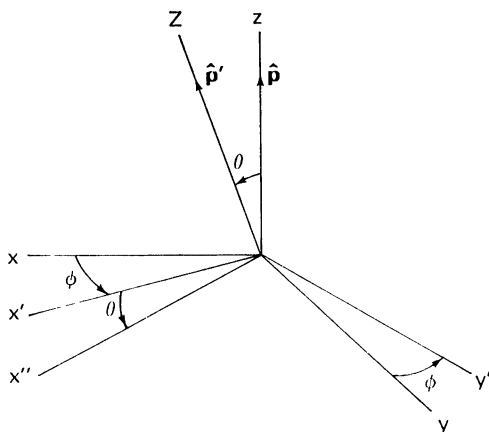


Fig. 18.2. The rotation of the coordinate system in which  $\hat{p} \equiv Oz$  into that in which  $\hat{p}' \equiv OZ$ .

Let us now consider the particular rotation through an angle  $\theta$  in the positive direction about the axis  $\mathbf{p} \times \mathbf{p}'$  (see Fig. 18.2). We want to switch from the "old" system of coordinates  $Oxyz$  into a new one  $OXYZ$  such that the new  $z$  axis  $OZ$  has the polar angles  $(\theta, \phi)$  in the old system. Examination of Figs. 18.1 and 18.2 shows that we must choose  $\alpha = \phi$  and  $\beta = \theta$ , but that the third

Euler angle  $\gamma$  is arbitrary. We shall take  $\gamma = -\phi$  (any other choice of  $\gamma$  amounts to a change of phase) so that

$$|p\theta\phi, \lambda\rangle = R_{\phi, \theta, -\phi} \psi_{p, \lambda} = e^{i\lambda\phi} R_{\phi, \theta, 0} \psi_{p, \lambda}. \quad (18.152)$$

Let us examine in detail how the operator  $R_{\alpha\beta\gamma}$  acts on a state  $|J, M\rangle$  which is an eigenket of the operators  $J^2$  and  $J_z$ , the corresponding eigenvalues being  $J(J+1)$  and  $M$  (with  $\hbar = 1$ ). If we suppress the other quantum numbers belonging to observables which commute with  $J^2$  and  $J_z$ , and use the fact that

$$[R_{\alpha\beta\gamma}, J^2] = 0 \quad (18.153)$$

we see that the matrix of  $R_{\alpha\beta\gamma}$  in the representation  $\{J, M\}$  is diagonal in  $J$ . Its elements are given by

$$\mathcal{D}_{M'M}^J(\alpha\beta\gamma) \equiv \langle JM' | R_{\alpha\beta\gamma} | JM \rangle = e^{-i\alpha M'} d_{M'M}^J(\beta) e^{-i\gamma M} \quad (18.154)$$

where the objects

$$d_{M'M}^J(\beta) = \langle JM' | \exp(-i\beta J_y) | JM \rangle \quad (18.155)$$

are called the *Wigner simplified rotation matrices*. Several important formulae for the  $d_{M'M}^J(\beta)$  are given in Appendix F.

We note that the matrix  $\mathcal{D}^J$  has dimensionality  $(2J+1)$ . It is called the  $(2J+1)$ -dimensional irreducible representation of the rotation group [31]. We may also write

$$R_{\alpha\beta\gamma} |JM\rangle = \sum_{M'} \mathcal{D}_{M'M}^J(\alpha\beta\gamma) |JM'\rangle. \quad (18.156)$$

We still have to specify the relative phases of the states  $\psi_{p\lambda}$  with momentum in the positive  $z$  direction. As a result of the statement iv) before eq. (18.146), we may construct the states  $\psi_{p\lambda}$  with  $\lambda$  fixed and a variable  $p$  by applying suitable *Lorentz-transformations* in the  $z$  direction to a fixed state  $\psi_{p_0\lambda}$ . For a particle having a *finite rest mass* this fixed state is conveniently chosen as the one corresponding to zero momentum ( $p_0 = 0$ ). Then, since for a particle at rest the angular momentum is precisely the spin it is possible to specify the relative phases of the states  $\psi_{p_0=0, \lambda}$  by the usual convention,

$$(J_x \pm iJ_y) \psi_{p_0=0, \lambda} = \sqrt{(s \mp \lambda)(s \pm \lambda + 1)} \psi_{p_0=0, \lambda \pm 1} \quad (18.157)$$

where  $J_x, J_y, J_z$  are the standard spin matrices.

For *massless particles* we cannot reduce  $p_0$  to zero by means of a finite Lorentz transformation. However, in this case there are only two possible helicity values to be compared, namely  $\lambda = \pm s$ . Owing to the statement iii) before eq. (18.146), this may be achieved by using a *reflection*. Consider for example a reflection in the  $x$ - $z$  plane such that the coordinates  $(x, y, z)$  of a point  $\mathbf{r}$  become  $(x, -y, z)$ . This may also be obtained by first applying the parity operator  $\mathcal{P}\mathbf{r} = -\mathbf{r}$  and then a rotation of  $180^\circ$  about the  $y$ -axis. Let

$$Y = \exp(-i\pi J_y) \mathcal{P} \quad (18.158)$$

be the operator describing this reflection in the  $(xz)$  plane. Then

$$Y\psi_{p,s} = \eta\psi_{p,-s} \quad (18.159)$$

and the “parity factor”  $\eta$  is independent of  $p$  because the operator  $Y$  commutes with a Lorentz transformation in the  $z$ -direction.

Let us verify that eq. (18.159) is compatible with the convention adopted above in the case  $m \neq 0$ . Then we know that

$$\mathcal{P}\psi_{0\lambda} = \eta\psi_{0\lambda} \quad (18.160)$$

where  $\eta$  is a phase factor independent of  $\lambda$  since  $\mathcal{P}$  commutes with  $\mathbf{J}$ . Moreover, since  $d_{M'M}^J(\pi) = (-)^{J-M}\delta_{M',-M}$  we have

$$\exp(-i\pi J_y)\psi_{0\lambda} = (-)^{s-\lambda}\psi_{0,-\lambda}. \quad (18.161)$$

We may then combine eqs. (18.160) and (18.161) and apply a Lorentz transformation up to momentum  $p$  in the  $z$  direction to obtain

$$Y\psi_{p\lambda} = \eta(-)^{s-\lambda}\psi_{p,-\lambda} \quad (18.162)$$

which for  $\lambda = s$  reduces to eq. (18.159).

Let us now consider *two* free particles 1 and 2 having masses  $m_1$  and  $m_2$  and spins  $s_1$  and  $s_2$ . The wave function for this system may be written as a direct product of the one-particle states considered above, namely

$$|p_1\theta_1\phi_1\lambda_1\rangle \times |p_2\theta_2\phi_2\lambda_2\rangle = R_{\phi_1,\theta_1,-\phi_1}^{(1)}\psi_{p_1\lambda_1} R_{\phi_2,\theta_2,-\phi_2}^{(2)}\psi_{p_2\lambda_2}. \quad (18.163)$$

Since we want to work in the C.M. system, we are interested in states of zero linear momentum ( $\mathbf{p}_1 + \mathbf{p}_2 = 0$ ). Let us call  $\mathbf{p} = \mathbf{p}_1 = -\mathbf{p}_2$  the relative momentum with polar coordinates  $(p\theta\phi)$ . Thus  $\theta_1 = \theta$ ,  $\phi_1 = \phi$ , while  $\theta_2 = \pi - \theta$ ,  $\phi_2 = \pi \pm \phi$ . The two rotations  $R^{(1)}$  and  $R^{(2)}$  may then be replaced by a single rotation generated by the total angular momentum  $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$  of the two particles, and acting on a basic state  $\psi_{p\lambda_1\lambda_2}$  such that  $\theta = \phi = 0$ . This state may be written as

$$\psi_{p\lambda_1\lambda_2} = \psi_{p\lambda_1}^{(1)} \chi_{p\lambda_2}^{(2)} \quad (18.164)$$

with

$$\chi_{p\lambda_2}^{(2)} = (-1)^{s_2-\lambda_2} \exp(-i\pi J_y^{(2)})\psi_{p\lambda_2}. \quad (18.165)$$

Here  $\chi_{p\lambda_2}^{(2)}$  represents a particle moving in the  $z$  direction, such that for a particle at rest ( $p = 0$ )  $\chi_{0\lambda_2}$  simply reduces to  $\psi_{0\lambda_2}$  with no additional phase factor. From the basic state  $\psi_{p\lambda_1\lambda_2}$  we may now generate the states with other directions of  $\mathbf{p}$  by applying a rotation. That is

$$|p\theta\phi, \lambda_1\lambda_2\rangle = R_{\phi,\theta,-\phi}\psi_{p\lambda_1\lambda_2} = e^{i\lambda\phi} R_{\phi,\theta,0}\psi_{p\lambda_1\lambda_2} \quad (18.166)$$

where  $\lambda = \lambda_1 - \lambda_2$  is the resultant angular momentum in the direction  $(\theta, \phi)$  of  $\mathbf{p}$ .

We now turn to the problem of constructing states with total angular momentum quantum number  $J$  and magnetic quantum number  $M$  (the eigenvalues of  $J_z$  being  $M$ ). Because the magnitude  $p$  of the vector  $\mathbf{p}$  and

the helicities  $\lambda_1$  and  $\lambda_2$  are invariant under rotations, we may use all the "good" quantum numbers  $p, J, M, \lambda_1, \lambda_2$  to label the state which we want to obtain. We shall write the corresponding ket as  $|p, J, M, \lambda_1, \lambda_2\rangle$ . Using the orthogonality relations satisfied by the rotation matrices, namely

$$\int_0^{2\pi} d\alpha \int_0^\pi d\beta \int_0^{2\pi} d\gamma \sin \beta \mathcal{D}_{M'\lambda'}^{J'*}(\alpha\beta\gamma) \mathcal{D}_{M\lambda}^J(\alpha\beta\gamma) = \frac{4\pi}{2J+1} \delta_{JJ'} \delta_{MM'} \quad (18.167)$$

one finds that

$$|p, J, M, \lambda_1, \lambda_2\rangle = \frac{N_J}{2\pi} \int_0^{2\pi} d\alpha \int_0^\pi d\beta \int_0^{2\pi} d\gamma \sin \beta \mathcal{D}_{M\lambda}^{J*}(\alpha\beta\gamma) R_{\alpha\beta\gamma} \psi_{p\lambda_1\lambda_2} \quad (18.168)$$

where  $N_J$  is a normalization factor. Let us adopt the normalization

$$\begin{aligned} \langle p'_1 p'_2 \lambda'_1 \lambda'_2 | p_1 p_2 \lambda_1 \lambda_2 \rangle &= \delta(\mathbf{P}' - \mathbf{0}) \delta(\mathbf{p}' - \mathbf{p}) \delta_{\lambda'_1 \lambda_1} \delta_{\lambda'_2 \lambda_2} \\ &= \delta(\mathbf{P}' - \mathbf{0}) \frac{1}{\rho(E)} \delta[E(p') - E(p)] \delta_{\mathbf{p}' \mathbf{p}} \delta_{\lambda'_1 \lambda_1} \delta_{\lambda'_2 \lambda_2} \end{aligned} \quad (18.169)$$

where  $\mathbf{P}' = \mathbf{p}'_1 + \mathbf{p}'_2$ ,  $\mathbf{p}$  and  $\mathbf{p}'$  are relative momenta,  $\rho = k^2 dk/dE$  and

$$\delta_{\mathbf{p}' \mathbf{p}} = \delta(\cos \theta - \cos \theta') \delta(\phi - \phi')$$

is the delta function on the unit sphere. Then, requiring that

$$\langle J' M' \lambda'_1 \lambda'_2 | J M \lambda_1 \lambda_2 \rangle = \delta_{JJ'} \delta_{MM'} \delta_{\lambda'_1 \lambda_1} \delta_{\lambda'_2 \lambda_2} \quad (18.170)$$

one easily shows [8] that  $N_J = (2J+1)/(4\pi)^{1/2}$ . Finally, we note that the transformation matrix from the linear to the angular momentum representation is given by

$$\langle \hat{\mathbf{p}} \lambda'_1 \lambda'_2 | J M \lambda_1 \lambda_2 \rangle = N_J \delta_{\lambda'_1 \lambda_1} \delta_{\lambda'_2 \lambda_2} \mathcal{D}_{M\lambda}^{J*}(\phi, \theta, -\phi). \quad (18.171)$$

Let us now express the  $S$  matrix in terms of helicity states. We consider a two-body reaction  $A + B \rightarrow C + D$  and write the  $S$  matrix element as

$$\langle p_C p_D \lambda_C \lambda_D | S | p_A p_B \lambda_A \lambda_B \rangle = \delta(\mathbf{P}_f - \mathbf{0}) \langle k_f \lambda_C \lambda_D | S | k_i \lambda_A \lambda_B \rangle \quad (18.172)$$

where  $\mathbf{P}_f = \mathbf{p}_C + \mathbf{p}_D$  while  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are respectively the relative momenta in the initial and final channel. We also define in the usual way

$$\langle k_f \lambda_C \lambda_D | S | k_i \lambda_A \lambda_B \rangle = [\rho_i \rho_f]^{-1/2} \delta[E_i(k_i) - E_f(k_f)] \langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | S | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle \quad (18.173)$$

with  $\rho_i = k_i^2 dk_i/dE_i$  and  $\rho_f = k_f^2 dk_f/dE_f$ . The  $T$ -matrix is defined by

$$\langle k_f \lambda_C \lambda_D | S | k_i \lambda_A \lambda_B \rangle = \delta_{ba} - 2\pi i \delta[E_i(k_i) - E_f(k_f)] \langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | T(k_i) | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle \quad (18.174)$$

where

$$\delta_{ba} = \delta_{AC} \delta_{BD} \delta(\mathbf{k}_f - \mathbf{k}_i).$$

We also note from eq. (18.173) that

$$\langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | S | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle = \delta_{ba} - 2\pi i (\rho_i \rho_f)^{1/2} \langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | T(k_i) | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle. \quad (18.175)$$

We may now transform to the  $\{J, M\}$  representation to obtain a *generalization partial wave expansion* for the  $S$ -matrix. Choosing the initial relative wave vector  $\mathbf{k}_i$  to lie along the  $z$  axis we first have

$$\begin{aligned}\langle JM\lambda_A\lambda_B|\theta_0 = 0, \phi_0, \lambda_A, \lambda_B\rangle &= N_J \mathcal{D}_{M\lambda}^{J*}(\phi_0, 0, -\phi_0) \\ &= N_J \exp\{i(M - \lambda)\phi_0\} d_{M\lambda}^J(0) \\ &= N_J \delta_{M\lambda}.\end{aligned}\quad (18.176)$$

We then have, using eqs. (18.171) and the fact that  $N_J = (2J + 1)/(4\pi)^{1/2}$ ,

$$\begin{aligned}\langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | S | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle &= \sum_{J, M} \langle \theta \phi \lambda_C \lambda_D | JM \lambda_C \lambda_D \rangle \langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle \langle JM \lambda_A \lambda_B | 00 \lambda_A \lambda_B \rangle \\ &= \sum_J \frac{2J + 1}{4\pi} \langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle \mathcal{D}_{\lambda\mu}^{J*}(\phi, \theta, -\phi)\end{aligned}\quad (18.177)$$

where  $(\theta_0 = \phi_0 = 0)$  are the polar angles of  $\mathbf{k}_i$ , and  $(\theta, \phi)$  are those of  $\mathbf{k}_f$ . We have also set  $\lambda = \lambda_A - \lambda_B$ ,  $\mu = \lambda_C - \lambda_D$  and we have used rotational invariance to write

$$\langle JM \lambda_C \lambda_D | S | J' M' \lambda_A \lambda_B \rangle = \delta_{JJ'} \delta_{MM'} \langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle. \quad (18.178)$$

We may simplify eq. (18.177) still further by using the relation

$$\mathcal{D}_{\lambda\mu}^{J*}(\phi, \theta, -\phi) = \exp\{i(\lambda - \mu)\phi\} d_{\lambda\mu}^J(\theta) \quad (18.179)$$

so that the *generalized partial wave expansion* of the  $S$  matrix takes the form

$$\langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | S | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle = \sum_J \frac{2J + 1}{4\pi} \langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle d_{\lambda\mu}^J(\theta) \exp\{i(\lambda - \mu)\phi\}. \quad (18.180)$$

This formula is the generalization of the expansion (18.61a) which we obtained for the case of spinless particles. We note that the generalized partial wave expansion (18.180) has a much simpler structure than the corresponding expansion (18.99) which we wrote above in the  $\{S, v\}$  representation. In particular, eq. (18.180) has only one summation index and does not involve Clebsch-Gordan coefficients. The only difficulty arises from the presence of the functions  $d_{\lambda\mu}^J$ ; a few of these functions are given in Appendix F.

A similar generalized partial wave expansion may be written for the  $T$ -matrix elements. That is

$$\langle \hat{\mathbf{k}}_f \lambda_C \lambda_D | T(k_i) | \hat{\mathbf{k}}_i \lambda_A \lambda_B \rangle = \sum_J \frac{2J + 1}{4\pi} \langle \lambda_C \lambda_D | T^J | \lambda_A \lambda_B \rangle d_{\lambda\mu}^J(\theta) \exp\{i(\lambda - \mu)\phi\} \quad (18.181)$$

so that, from eqs. (18.175) and (18.180), we deduce that

$$\langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle = \delta_{AC} \delta_{BD} \delta_{\lambda_A \lambda_C} \delta_{\lambda_B \lambda_D} - 2\pi i (\rho_i \rho_f)^{1/2} \langle \lambda_C \lambda_D | T^J | \lambda_A \lambda_B \rangle. \quad (18.182)$$

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \rho_f |\langle \hat{k}_f \lambda_C \lambda_D | T(k_i) | \hat{k}_i \lambda_A \lambda_B \rangle|^2 \quad (18.183a)$$

or

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{k_i^2} \rho_i \rho_f |\langle \hat{k}_f \lambda_C \lambda_D | T(k_i) | \hat{k}_i \lambda_A \lambda_B \rangle|^2. \quad (18.183b)$$

We may also define a *scattering amplitude*  $f_{\lambda_C \lambda_D; \lambda_A \lambda_B}(\theta, \phi)$  by the relation

$$f_{\lambda_C \lambda_D; \lambda_A \lambda_B}(\theta, \phi) = -(2\pi)^2 \left( \frac{\rho_i \rho_f}{k_i k_f} \right)^{1/2} \langle \hat{k}_f \lambda_C \lambda_D | T(k_i) | \hat{k}_i \lambda_A \lambda_B \rangle \quad (18.184)$$

so that the differential cross section is given by [see eq. (15.49)]

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} |f_{\lambda_C \lambda_D; \lambda_A \lambda_B}|^2. \quad (18.185)$$

We note from eqs. (18.181) and (18.185) that

$$f_{\lambda_C \lambda_D; \lambda_A \lambda_B}(\theta, \phi) = -\pi \left( \frac{\rho_i \rho_f}{k_i k_f} \right)^{1/2} \sum_J (2J+1) \langle \lambda_C \lambda_D | T^J | \lambda_A \lambda_B \rangle \times d_{\lambda\mu}^J(\theta) \exp\{i(\lambda - \mu)\phi\}. \quad (18.186)$$

Using eq. (18.182) we may also write

$$f_{\lambda_C \lambda_D; \lambda_A \lambda_B}(\theta, \phi) = \frac{1}{2i(k_i k_f)^{1/2}} \sum_J (2J+1) \{ \langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle - \delta_{AC} \delta_{BD} \delta_{\lambda_A \lambda_C} \delta_{\lambda_B \lambda_D} \} d_{\lambda\mu}^J(\theta) \exp\{i(\lambda - \mu)\phi\}. \quad (18.187)$$

This last relation is obviously a direct generalization of the familiar formula for spinless particles, namely

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [S_l(k) - 1] P_l(\cos \theta) \quad (18.188)$$

with  $S_l(k) = \exp[2i\delta_l(k)]$ .

#### 18.2.4. The role of invariance principles

We have already seen in section 16.7 how symmetry principles imply some remarkable relations which simplify the determination of the  $S$ -matrix. This will now be illustrated on two-body scattering.

We first note that we have only used the invariance with respect to *space-time translations* (conservation of total momentum and energy) together with *rotational invariance* to obtain the expansions (18.99) or (18.180).

Let us suppose in addition that *parity* is conserved, and analyze the influence of this symmetry principle on the matrix elements  $\langle l'S' | S^J | lS \rangle$  appearing in the expansion (18.99). In this case the orbital angular momenta  $l$  and  $l'$  must be simultaneously even or odd, so that no transition from an even (odd) to an odd (even) state of angular momentum may occur. For

example, consider the elastic scattering of two particles having respectively spin  $\frac{1}{2}$  and spin 0. In this case the total spin is  $S = \frac{1}{2}$ , and the only possible values of the orbital angular momentum (for a given  $J$ ) are  $l = J \pm \frac{1}{2}$ . If parity is conserved, we see that no transition can occur between the states with  $l = J + \frac{1}{2}$  and those with  $l = J - \frac{1}{2}$ . Hence we must have  $l = l'$ .

As another example of the influence of parity conservation, consider the case of two particles of spin  $\frac{1}{2}$ . Then  $S$  and  $S'$  can only be zero or unity. For  $S = 0$ , we must have  $l = J$ ; for  $S = 1$ , we may have  $l = J, J + 1, J - 1$ . If parity is conserved, no transition can occur between the states of parity  $(-)^J$  and those of parity  $(-)^{J+1}$ . Hence the states with  $l = J$  are "decoupled" from the others. The former states correspond to  $l = l' = J$  with  $S$  and  $S'$  being either 0 or 1. The latter are such that  $l = J \pm 1, l' = J \pm 1$  with  $S = S' = 1$ .

TABLE 18.1  
The first states of the nucleon-nucleon system allowed by  
the generalized Pauli principle

$J$	$I = 0$		$I = 1$	
	$S = 0$	$S = 1$	$S = 0$	$S = 1$
0	—	—	$^1S_0$	$^3P_0$
1	$^1P_1$	$^3S_1$ $^3D_1$	—	$^3P_1$
2	—	$^3D_2$	$^1D_2$	$^3P_2$ $^3F_2$
3	$^1F_3$	$^3D_3$ $^3G_3$	—	$^3F_3$

Further important symmetry arises when the two particles are *identical*, in which case eq. (18.99) or (18.180) must be symmetrized. This, in general, will eliminate certain states from the sums in eq. (18.99) or (18.180). Similar considerations apply when *isotopic spin* symmetries must be taken into account. For example, let us consider the *nucleon-nucleon* system which may have total spin  $S = 0$  or  $S = 1$  and total isotopic spin  $I = 0$  or  $I = 1$ . In this case the (generalized) Pauli principle states that the total wave function of the system, which is a product of an orbital, a spin and an isospin part must be totally antisymmetric. The allowed states of the system are then easily constructed, the first of them being given in Table 18.1 in the Russell-Saunders notation [32]  $^{2S+1}L_J$ . We also note that if the Hamiltonian of the nucleon-nucleon system commutes [33] with  $I^2$  (the square of the total isotopic spin operator) so that  $I$  is a good quantum number, then parity conservation and the generalized exclusion principle imply that singlet-triplet transitions are strictly forbidden. Hence we also have  $[H, S^2] = 0$  in this case.

Another important simplification of eq. (18.99) arises when the condition of *time reversal invariance* holds. In this case it can be shown [34] that the matrix  $\langle l'S'|S^J|lS \rangle$  is *symmetric*. That is

$$\langle l'S'|S^J|lS \rangle = \langle lS|S^J|l'S' \rangle. \quad (18.189)$$



The unitarity of the  $S$ -matrix together with the symmetry relation (18.189), implies that  $S$  may be diagonalized by an orthogonal, real matrix  $A$ . Thus

$$\langle l'S'|S^J|lS\rangle = \sum_{\alpha} \langle l'S'|A^J|\alpha\rangle \exp(2i\delta_{\alpha}^J) \langle \alpha|A^J|lS\rangle \quad (18.190)$$

where the quantities  $\delta_{\alpha}^J$  are called the *eigenphase shifts*. Because the  $S$ -matrix is unitary, the eigenphase shifts are real.

As an example, let us return again to the nucleon-nucleon system. In the singlet state ( $S = 0$ ) one has  $l = l' = J$  and the submatrix  $\langle l', 0|S^J|l, 0\rangle$  is already diagonal. In the triplet state one has  $S = 1$  so that, for a given value of  $J$ , we have  $l = J - 1, J, J + 1$ . If we write the corresponding submatrix as a  $3 \times 3$  matrix whose elements are labeled by the indices  $l, l' = J - 1, J, J + 1$  we see from *parity conservation* that this matrix must have the form

$$\langle l', 1|S^J|l, 1\rangle \equiv S_{l'l}^J = \begin{bmatrix} S_{J-1, J-1}^J & 0 & S_{J-1, J+1}^J \\ 0 & S_{JJ}^J & 0 \\ S_{J+1, J-1}^J & 0 & S_{J+1, J+1}^J \end{bmatrix}. \quad (18.191)$$

We note that this matrix is non-diagonal since in general the interaction mixes the states  $l = J - 1$  and  $l = J + 1$ . The unitarity condition implies that  $|S_{JJ}^J|^2 = 1$ , so that we may write immediately

$$S_{JJ}^J = \exp\{2i\delta_J^J(k)\} \quad (18.192)$$

a relation which defines the real phase shifts  $\delta_J^J$  corresponding to the transitions ( $S = 1, l = J$ )  $\rightarrow$  ( $S = 1, l = J$ ), (i.e. to the states  ${}^3P_1, {}^3D_2, {}^3F_3$ , etc.).

Let us now express that the  $2 \times 2$  submatrix  $S_{l'l}^J$ , corresponding to the values  $l, l' = J \pm 1$  is unitary and symmetric. Such a matrix depends on 3 real parameters [35]. Following eq. (18.190) we may write (for  $S = S' = 1$ )

$$S_{l'l}^J = \sum_{\alpha=1,2} A_{l'\alpha}^J \exp(2i\delta_{\alpha}^J) A_{\alpha l}^J \quad (18.193)$$

and choose [14]

$$A_{l'\alpha}^J = \begin{bmatrix} \cos \varepsilon_J & \sin \varepsilon_J \\ -\sin \varepsilon_J & \cos \varepsilon_J \end{bmatrix} \quad (18.194)$$

where the quantity  $\varepsilon_J$  is called the *mixing parameter*. Hence the  $2 \times 2$  submatrix  $S_{l'l}^J$  of eq. (18.193) becomes

$$S_{l'l}^J = \begin{bmatrix} \cos^2 \varepsilon_J \exp(2i\delta_1^J) + \sin^2 \varepsilon_J \exp(2i\delta_2^J) & \frac{1}{2} \sin 2\varepsilon_J [\exp(2i\delta_1^J) - \exp(2i\delta_2^J)] \\ \frac{1}{2} \sin 2\varepsilon_J [\exp(2i\delta_1^J) - \exp(2i\delta_2^J)] & \sin^2 \varepsilon_J \exp(2i\delta_1^J) + \cos^2 \varepsilon_J \exp(2i\delta_2^J) \end{bmatrix}. \quad (18.195)$$

We note that when  $\varepsilon_J = 0$  this submatrix is diagonal and the entire problem reduces to scattering by central forces.

We now consider briefly the effect of invariance principles on the  $S$ -matrix elements expressed in terms of helicity states [see eq. (18.180)]. Firstly, if *parity is conserved*, one finds that [8]

$$\langle -\lambda_C, -\lambda_D | S^J | -\lambda_A, -\lambda_B \rangle = (-1)^{S_C + S_D - S_A - S_B} \frac{\zeta_C \zeta_D}{\zeta_A \zeta_B} \langle \lambda_C \lambda_D | S^J | \lambda_A \lambda_B \rangle \quad (18.196)$$

and

$$f_{-\lambda_C - \lambda_D; -\lambda_A, -\lambda_B}(\theta, \phi) = (-1)^{S_C + S_D - S_A - S_B} \frac{\zeta_C \zeta_D}{\zeta_A \zeta_B} f_{\lambda_C \lambda_D; \lambda_A \lambda_B}(\theta, \pi - \phi) \quad (18.197)$$

where  $\zeta_A, \zeta_B, \dots$  are the intrinsic parities of the particles [see eq. (16.196)].

Let us illustrate eq. (18.196) on the simple case of elastic spin  $\frac{1}{2}$ -spin 0 scattering, for example elastic pion-nucleon scattering. In this case we have only four helicity amplitudes to consider, namely

$$\begin{aligned} \langle + | S^J | + \rangle &\equiv S_{++}^J, & \langle - | S^J | + \rangle &\equiv S_{-+}^J \\ \langle + | S^J | - \rangle &\equiv S_{+-}^J, & \langle - | S^J | - \rangle &\equiv S_{--}^J \end{aligned} \quad (18.198)$$

where the indices  $\lambda_B, \lambda_D$  have been suppressed and we use for  $\lambda_A$  and  $\lambda_C$  the notation  $\pm$  instead of  $\pm \frac{1}{2}$ . Hence parity conservation, expressed by eq. (18.196), implies that

$$S_{++}^J = S_{--}^J, \quad S_{+-}^J = S_{-+}^J. \quad (18.199)$$

We note here a drawback of the helicity formalism. Since the basic helicity states are not eigenstates of parity, we must form linear combinations of the helicity states to diagonalize the  $S$ -matrix. In this example, the states

$$\frac{1}{\sqrt{2}} [|JM+\rangle + |JM-\rangle] \quad (18.200a)$$

and

$$\frac{1}{\sqrt{2}} [|JM+\rangle - |JM-\rangle] \quad (18.200b)$$

may easily be shown to have respectively the parities  $(-)^{J-1/2}$  and  $(-)^{J+1/2}$ . The first state (18.200a) therefore corresponds to the state with  $l = J - \frac{1}{2}$  in the  $\{L, S\}$  representation, while the state (18.200b) corresponds to that with  $l = J + \frac{1}{2}$ . Now we have already shown above that if parity is conserved the states  $l = J - \frac{1}{2}$  decouple from those with  $l = J + \frac{1}{2}$  and that  $l = l'$ . Hence we may write directly

$$S_{l'l}^{J=l+1/2} = \exp(2i\delta_{l+}) \quad (18.201a)$$

and

$$S_{ll}^{J=l-1/2} = \exp(2i\delta_{l-}). \quad (18.201b)$$

Thus, using eqs. (18.199)–(18.201), we find that the state (18.200a) has the phase shift  $\delta_{l+}$  with  $l = J - \frac{1}{2}$ , while the state (18.200b) has the phase shift  $\delta_{l'-}$ , with  $l' = J + \frac{1}{2} = l + 1$ . Therefore the diagonal  $S$ -matrix elements are

$$S_{++}^J + S_{+-}^J = \exp(2i\delta_{l+}) \quad (18.202a)$$

and

$$S_{++}^J - S_{+-}^J = \exp(2i\delta_{(l+1)-}). \quad (18.202b)$$

Let us now examine how the symmetrization required by the presence of *identical particles* affects the helicity amplitudes. If  $P_{12}$  is the operator which interchanges the particles 1 and 2 we have

$$P_{12}\psi_{p\lambda_1\lambda_2} = (-1)^{2s-\lambda_1+\lambda_2} \exp(i\pi J_y)\psi_{p\lambda_2\lambda_1} \quad (18.203)$$

where we have used eqs. (18.164) and (18.165), together with the fact that

$$\exp(-i\pi J_y^{(1)}) = (-1)^{2s} \exp(i\pi J_y^{(1)})$$

and

$$(-1)^{\lambda_1-\lambda_2} = (-1)^{\lambda_2-\lambda_1}$$

since  $\lambda_1 - \lambda_2$  is an integer when particles 1 and 2 are identical.

Because  $P_{12}$  commutes with the rotation operators, we may investigate the effect of  $P_{12}$  on a state  $|JM\lambda_1\lambda_2\rangle$ . The result is

$$P_{12}|JM\lambda_1\lambda_2\rangle = (-1)^{J-2s}|JM\lambda_2\lambda_1\rangle \quad (18.204)$$

so that the states which are correctly symmetrized with respect to  $P_{12}$  are

$$\{1 + (-1)^{2s}P_{12}\}|JM\lambda_1\lambda_2\rangle = |JM\lambda_1\lambda_2\rangle + (-1)^J|JM\lambda_2\lambda_1\rangle. \quad (18.205)$$

We note that when  $J$  is odd only the states with  $\lambda_1 \neq \lambda_2$  are allowed [36].

Finally, we examine the consequences of *time reversal invariance*. We note that under this operation the helicities of the particles are left unchanged, since both spin and momentum are changed. The direction of relative motion being reversed, we have

$$\mathcal{K}|\theta\phi\lambda_1\lambda_2\rangle = |\pi - \theta, \phi + \pi, \lambda_1\lambda_2\rangle \quad (18.206)$$

where  $\mathcal{K}$  is the operator of time reversal (see Section 16.7). From this equation one may deduce that

$$\mathcal{K}|JM\lambda_1\lambda_2\rangle = (-1)^{J+M}|JM\lambda_1\lambda_2\rangle \quad (18.207)$$

together with the symmetry property

$$\langle\lambda_C\lambda_D|S^J|\lambda_A\lambda_B\rangle = \langle\lambda_A\lambda_B|S^J|\lambda_C\lambda_D\rangle \quad (18.208)$$

which is the analogue of eq. (18.189).

### 18.3. Scattering of spin zero by spin one-half particles

We now examine in some detail the simplest example of scattering by non-central forces, namely the scattering of spin zero by spin one-half particles. Important applications include pion-nucleon scattering and the scattering of spin one-half hadrons by spin zero nuclei.

#### 18.3.1. General formulae

In the case of spin 0–spin  $\frac{1}{2}$  scattering we always have  $S = S' = \frac{1}{2}$ . Hence, for a given state of total angular momentum  $J$  the orbital angular momentum  $l$  may take the values  $l = J + \frac{1}{2}$  or  $l = J - \frac{1}{2}$ . We must therefore consider four matrix elements of the type  $\langle l'S'|S^J|lS\rangle$ , namely

$$\begin{aligned} \langle J + \tfrac{1}{2}, \tfrac{1}{2}|S^J|J + \tfrac{1}{2}, \tfrac{1}{2}\rangle &\equiv S_{J+1/2, J+1/2}^J, \\ \langle J - \tfrac{1}{2}, \tfrac{1}{2}|S^J|J - \tfrac{1}{2}, \tfrac{1}{2}\rangle &\equiv S_{J-1/2, J-1/2}^J, \\ \langle J - \tfrac{1}{2}, \tfrac{1}{2}|S^J|J + \tfrac{1}{2}, \tfrac{1}{2}\rangle &\equiv S_{J-1/2, J+1/2}^J, \\ \langle J + \tfrac{1}{2}, \tfrac{1}{2}|S^J|J - \tfrac{1}{2}, \tfrac{1}{2}\rangle &\equiv S_{J+1/2, J-1/2}^J. \end{aligned} \quad (18.209)$$

Let us assume that *parity is conserved*. Then, as we have shown in Section 18.2.4,

$$\langle l', \tfrac{1}{2}|S^J|l, \tfrac{1}{2}\rangle = \delta_{l'l} S_{l'l}^J \quad (18.210)$$

so that the two last  $S$ -matrix elements of (18.209) vanish. Hence the  $S$ -matrix is already diagonal and the first two matrix elements of (18.209) are those given in eq. (18.201), namely

$$S_{l'l}^{J=l+1/2} = \exp(2i\delta_{l+}) \quad \text{and} \quad S_{l'l}^{J=l-1/2} = \exp(2i\delta_{l-}).$$

We may now use the generalized partial wave expansion of the  $S$  matrix [eq. (18.99)] together with eq. (18.210) to write

$$\langle \hat{k}_f \tfrac{1}{2} v' | S(k) | \hat{k}_i \tfrac{1}{2} v \rangle = \sum_{l,J} \langle \hat{k}_f l \tfrac{1}{2} v' | \mathcal{Q}^J | \hat{k}_i l \tfrac{1}{2} v \rangle S_{ll}^J. \quad (18.211)$$

Similarly, using the generalized partial wave expansion (18.101) of the  $T$  matrix, together with the definition (18.94) and eq. (18.102), we have

$$\langle \hat{k}_f \tfrac{1}{2} v' | T(k) | \hat{k}_i \tfrac{1}{2} v \rangle = \sum_{lm'm'JM} Y_{lm'}(\hat{k}_f) Y_{lm}^*(\hat{k}_i) \langle l \tfrac{1}{2} m' v' | JM \rangle \langle l \tfrac{1}{2} m v | JM \rangle T_{ll}^J \quad (18.212)$$

where

$$T_{ll}^J = \frac{1}{2\pi i \rho(E)} (1 - S_{ll}^J). \quad (18.213)$$

Using the notation introduced in eqs. (18.201) it is also useful to define

$$T_{l'l}^{J=l\pm 1/2} = T_{l\pm} = \frac{1}{2\pi i \rho(E)} [1 - \exp(2i\delta_{l\pm})] = -\frac{1}{\pi \rho(E)} \exp(i\delta_{l\pm}) \sin \delta_{l\pm}. \quad (18.214)$$

Once the phase shifts have been evaluated, it is a simple matter to compute the  $T$ -matrix elements (18.212) and therefore the cross section (18.103).

Before we turn to the explicit evaluation of the phase shifts  $\delta_{l\pm}$  in the case of non-relativistic scattering by a given potential, let us ask what is the most general form of the scattering matrix for spin zero–spin  $\frac{1}{2}$  scattering. To this end, let us return to the generalized scattering amplitude  $M$  introduced in eqs. (18.112)–(18.113). In the case considered here ( $S = S' = \frac{1}{2}$ ) it has matrix elements

$$\langle \chi_{1/2, v'} | M | \chi_{1/2, v} \rangle = -(2\pi)^2 k \frac{dk}{dE} \langle \hat{k}_f \frac{1}{2} v' | T(k) | \hat{k}_i \frac{1}{2} v \rangle \quad (18.215)$$

and is clearly a matrix acting in two-dimensional spin space. As in Section 15.5.2 we now observe that the unit matrix

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and the three Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (18.216)$$

are a complete set of  $2 \times 2$  matrices [37]. We may therefore write the matrix  $M$  as

$$M = A I + \sum_{i=1}^3 \sigma_i B_i \quad (18.217)$$

where the coefficients  $A, B_1, B_2, B_3$  are complex numbers.

If the interaction is rotationally invariant,  $M$  is a scalar. Then the coefficients  $B_i$  must be the components of a vector  $\mathbf{B}$ , and we may write eq. (18.217) as

$$M = A I + \boldsymbol{\sigma} \cdot \mathbf{B}. \quad (18.218)$$

The only independent vectors which can be constructed from  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are  $\mathbf{k}_i \times \mathbf{k}_f$  and  $\mathbf{k}_i \pm \mathbf{k}_f$ . We may therefore write the most general form of  $M$  compatible with *rotational invariance* as

$$M = A I + b_1 \boldsymbol{\sigma} \cdot (\mathbf{k}_i \times \mathbf{k}_f) + b_2 \boldsymbol{\sigma} \cdot (\mathbf{k}_i + \mathbf{k}_f) + b_3 \boldsymbol{\sigma} \cdot (\mathbf{k}_i - \mathbf{k}_f) \quad (18.219)$$

where the coefficients  $A, b_1, b_2, b_3$  are functions of  $k = |\mathbf{k}_i| = |\mathbf{k}_f|$  and of the scattering angle  $\theta$ .

Let us examine the effect of *parity conservation* on eq. (18.219). Using eqs. (16.186) we see that when the parity operation is performed

$$\begin{aligned} \mathcal{P}(\mathbf{k}_i + \mathbf{k}_f) \mathcal{P}^\dagger &= -(\mathbf{k}_i + \mathbf{k}_f) \\ \mathcal{P}(\mathbf{k}_i \times \mathbf{k}_f) \mathcal{P}^\dagger &= \mathbf{k}_i \times \mathbf{k}_f \\ \mathcal{P} \boldsymbol{\sigma} \mathcal{P}^\dagger &= \boldsymbol{\sigma}. \end{aligned} \quad (18.220)$$

Hence, invariance under space reflection rules out the two last terms in eq. (18.219). We may then write the matrix  $M$  (using a slightly different notation) as

$$M = f(k, \theta) + \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} g(k, \theta) \quad (18.221)$$

where the unit matrix  $I$  is implied in the first term and  $\hat{\mathbf{n}}$  is the axial unit vector perpendicular to the scattering plane, namely

$$\hat{\mathbf{n}} = \frac{\mathbf{k}_i \times \mathbf{k}_f}{|\mathbf{k}_i \times \mathbf{k}_f|} = \frac{\hat{\mathbf{k}}_i \times \hat{\mathbf{k}}_f}{\sin \theta}, \quad \cos \theta = \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f. \quad (18.222)$$

In order to compute the scattering amplitudes  $f$  and  $g$  we must know the Hamiltonian of the system. We note that the first term in eq. (18.221) cannot induce any change in the spin state of the particles, while the second term may; the amplitude  $g$  is therefore frequently called the “spin-flip” amplitude.

It is also interesting to ask about the effect of *time-reversal invariance* on the expression of  $M$ . Assuming always rotational invariance, so that eq. (18.219) holds, one may use the reciprocity theorem (16.239) to infer that the last term in eq. (18.219) must be omitted when time reversal invariance holds. Hence the most general expression of  $M$ , valid under the assumptions of invariance with respect to rotations and time reversal, is

$$M = A I + b_1 \boldsymbol{\sigma} \cdot (\mathbf{k}_i \times \mathbf{k}_f) + b_2 \boldsymbol{\sigma} \cdot (\mathbf{k}_i + \mathbf{k}_f). \quad (18.223)$$

We note that this expression is less restrictive than the form (18.221) imposed by rotational invariance and parity conservation. In what follows we shall assume that parity is conserved and use only the expression (18.221).

### 18.3.2. *Non-relativistic scattering*

Let us now particularize our discussion to *non-relativistic* spin 0–spin  $\frac{1}{2}$  scattering. We must then solve the Schrödinger equations (18.133) which in our case are *uncoupled* since we assume parity conservation. This, of course, requires the knowledge of the quantities  $\mathcal{V}_H^I$  or, in other words, of the interaction potential  $V$ . We shall suppose here that  $V$  has the form

$$V = V_c(r) + V_s(r) \boldsymbol{\sigma} \cdot \mathbf{L} \quad (18.224)$$

where  $V_c$  and  $V_s$  are called respectively the central part of the potential and its spin–orbit part; we shall assume that  $V_c$  and  $V_s$  both depend only on  $r = |\mathbf{r}|$ . We recall that  $\mathbf{L}$ , as given by eq. (18.6), is the orbital angular momentum of the two particles, in their C.M. system. We note that the potential  $V$  of eq. (18.224), and hence the full Hamiltonian of the system, is invariant under rotations and space reflections (i.e. conserves parity) [38]. A spin–orbit coupling of the form given in eq. (18.224) was first encountered in atomic physics, where it arises from relativistic corrections due to the interaction of an electron’s spin with its orbital angular momentum. Whereas the spin–orbit part of the potential (18.224) leads to small corrections in atomic structure, it plays a much more important role in nuclear phenomena.

With the interaction potential given by eq. (18.224), the total Hamiltonian of the system may be written in the coordinate representation as

$$H = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V_c(r) + V_s(r)\boldsymbol{\sigma}\cdot\mathbf{L} \quad (18.225)$$

where  $m = m_A m_B / (m_A + m_B)$  is the reduced mass of the two colliding particles. The Schrödinger equation satisfied by the scattering wave function  $\Psi_{\mathbf{k}_i, 1/2, v}^{(+)}$  is then

$$\left[ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2} + k^2 - U_c(r) - U_s(r)\boldsymbol{\sigma}\cdot\mathbf{L} \right] \Psi_{\mathbf{k}_i, 1/2, v}^{(+)} = 0 \quad (18.226)$$

where the reduced potentials  $U_c$  and  $U_s$  are given by

$$U_c(r) = \frac{2m}{\hbar^2} V_c(r); \quad U_s(r) = \frac{2m}{\hbar^2} V_s(r). \quad (18.227)$$

Let us analyze  $\Psi_{\mathbf{k}_i, 1/2, v}^{(+)}$  in partial waves according to eq. (18.119b). In this case we simply have

$$\Psi_{\mathbf{k}_i, 1/2, v}^{(+)} = (2/\pi)^{1/2} \sum_{l, j, v'} i^l \langle \hat{\mathbf{r}} l \frac{1}{2} v' | \mathcal{Y}^J | \hat{\mathbf{k}}_i l \frac{1}{2} v \rangle R_l^J(k, r) \chi_{1/2, v}. \quad (18.228)$$

Before we substitute this expansion in eq. (18.226) we note that since  $\mathbf{J} = \mathbf{L} + \frac{1}{2}\boldsymbol{\sigma}$  we may write

$$\boldsymbol{\sigma}\cdot\mathbf{L} = J^2 - L^2 - \frac{1}{4}\boldsymbol{\sigma}^2$$

where we have set  $\hbar = 1$ . Hence

$$\boldsymbol{\sigma}\cdot\mathbf{L} |l \frac{1}{2} J M\rangle = l |l \frac{1}{2} J M\rangle, \quad J = l + \frac{1}{2} \quad (18.229a)$$

and

$$\boldsymbol{\sigma}\cdot\mathbf{L} |l \frac{1}{2} J M\rangle = -(l+1) |l \frac{1}{2} J M\rangle, \quad J = l - \frac{1}{2}. \quad (18.229b)$$

Hence, defining the quantities

$$\begin{aligned} U_{l+}(r) &= U_c(r) + l U_s(r), \\ U_{l-}(r) &= U_c(r) - (l+1) U_s(r), \end{aligned} \quad (18.230)$$

we find that the radial functions  $R_l^J(k, r)$  satisfy the equations

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 - U_{l\pm}(r) \right] R_{l\pm}(k, r) = 0 \quad (18.231)$$

where we have written  $R_{l+} \equiv R_l^{J=l+1/2}$  and  $R_{l-} \equiv R_l^{J=l-1/2}$ .

We see that the original problem is reduced to the solution of two uncoupled radial equations whose form is exactly the same as eq. (4.15). We may therefore directly apply the methods of Chapter 4 to these equations, remembering that the central potential  $U_{l+}$  governs the scattering in the (+) states, while the other central potential  $U_{l-}$  corresponds to the (−) states. In particular, we may simplify eqs. (18.231) by introducing the new radial functions

$$u_{l\pm}(k, r) = A_{l\pm}(k) r R_{l\pm}(k, r) \quad (18.232)$$

where  $A_{l\pm}(k)$  depends on the "normalization" which we adopt. Then eqs. (18.231) become

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U_{l\pm}(r) \right] u_{l\pm}(k, r) = 0 \quad (18.233)$$

and if we choose  $A_{l\pm}(k) = \exp[i\delta_{l\pm}(k)]/k$ , we find that

$$u_{l\pm}(k, r) \xrightarrow{r \rightarrow \infty} \sin(kr - \frac{1}{2}l\pi + \delta_{l\pm}). \quad (18.234)$$

With the phase shifts  $\delta_{l\pm}$  obtained from the solution of eqs. (18.233) we may construct the quantities  $T_{l\pm}$  of eq. (18.214) and therefore the  $T$  matrix elements (18.212) and the cross sections. Another possibility consists in writing [see eq. (18.116)]

$$\Psi_{\mathbf{k}_i, \mathbf{v}}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_i \cdot \mathbf{r}) \chi_{\mathbf{v}} + \frac{e^{ikr}}{r} \sum_{\mathbf{v}'} \langle \mathbf{v}' | M | \mathbf{v} \rangle \chi_{\mathbf{v}'} \right] \quad (18.235)$$

where the matrix  $M$  is given by eq. (18.221) and we have omitted the indices referring to  $S = S' = \frac{1}{2}$ . Then, according to eq. (18.117), we have for a transition  $(\mathbf{k}_i, \mathbf{v}) \rightarrow (\mathbf{k}_f, \mathbf{v}')$

$$\frac{d\sigma}{d\Omega}(\mathbf{v} \rightarrow \mathbf{v}') = |\langle \mathbf{v}' | M | \mathbf{v} \rangle|^2. \quad (18.236)$$

In this case we need the expressions of the amplitudes  $f$  and  $g$  in terms of the phase shifts  $\delta_{l\pm}$ . A simple generalization of the partial wave method, using the operators

$$A_{l+} = \frac{l+1 + \boldsymbol{\sigma} \cdot \mathbf{L}}{2l+1}, \quad (18.237)$$

$$A_{l-} = \frac{l - \boldsymbol{\sigma} \cdot \mathbf{L}}{2l+1} \quad (18.238)$$

which project respectively onto the states  $J = l \pm \frac{1}{2}$ , yields the result

$$M = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [\{\exp(2i\delta_{l+}) - 1\} A_{l+} + \{\exp(2i\delta_{l-}) - 1\} A_{l-}] P_l(\cos \theta) \quad (18.239)$$

where we recall that

$$\exp(2i\delta_{l\pm}) = S_{ll}^{J=l \pm 1/2}. \quad (18.240)$$

Introducing the explicit form of  $A_{l\pm}$ , we then have

$$M = \frac{1}{2ik} \sum_{l=0}^{\infty} [(l+1)\{\exp(2i\delta_{l+}) - 1\} + l\{\exp(2i\delta_{l-}) - 1\}] P_l(\cos \theta) \\ + \frac{1}{2ik} \sum_{l=0}^{\infty} [\exp(2i\delta_{l+}) - \exp(2i\delta_{l-})] \boldsymbol{\sigma} \cdot \mathbf{L} P_l(\cos \theta). \quad (18.241)$$



Now

$$LP_l(\cos \theta) = (-i\mathbf{k}_r \times \nabla_{\mathbf{k}_r} P_l(\cos \theta) = i\hat{\mathbf{n}} \sin \theta P'_l(\cos \theta) \quad (18.242)$$

where  $\hat{\mathbf{n}}$  is the unit vector defined by eq. (18.222) and  $P'_l(\cos \theta) = dP_l(\cos \theta)/d(\cos \theta)$ . Hence, using eqs. (18.221), (18.241) and (18.242), we find that

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} [(l+1)\{\exp(2i\delta_{l+}) - 1\} + l\{\exp(2i\delta_{l-}) - 1\}] P_l(\cos \theta) \quad (18.243)$$

and

$$g(k, \theta) = \frac{\sin \theta}{2k} \sum_{l=1}^{\infty} [\exp(2i\delta_{l+}) - \exp(2i\delta_{l-})] P'_l(\cos \theta). \quad (18.244)$$

We note incidentally that eqs. (18.243) and (18.244) are equally valid when the potentials  $V_c(r)$  and (or)  $V_s(r)$  are complex [39], in which case the phase shifts  $\delta_{l\pm}$  are complex and we may write (see Section 4.6)

$$\exp\{2i[\text{Re } \delta_{l\pm} + i \text{Im } \delta_{l\pm}]\} = \eta_{l\pm} \exp(2i \text{Re } \delta_{l\pm}) \quad (18.245)$$

where

$$\eta_{l\pm} = \exp(-2 \text{Im } \delta_{l\pm}) \quad (18.246)$$

are “inelasticity” or “absorption” factors. We may also write eqs. (18.243)–(18.244) as

$$f(k, \theta) = \frac{1}{k} \sum_{l=0}^{\infty} [(l+1)\exp(i\delta_{l+}) \sin \delta_{l+} + l\exp(i\delta_{l-}) \sin \delta_{l-}] P_l(\cos \theta) \quad (18.247)$$

and

$$g(k, \theta) = \frac{i}{k} \sum_{l=1}^{\infty} [\exp(i\delta_{l+}) \sin \delta_{l+} - \exp(i\delta_{l-}) \sin \delta_{l-}] P'_l(\cos \theta) \quad (18.248)$$

where we have used the fact that [see eq. (B.9) of Appendix B]

$$P_l^1(\cos \theta) = \sin \theta P'_l(\cos \theta).$$

We note that unless the sum in eq. (18.248) is singular at  $\theta = 0$ , the “spin flip” amplitude  $g$  vanishes in the forward direction.

We also remark that in the absence of spin-orbit forces ( $V_s = 0$ ) we have

$$\exp(2i\delta_{l+}) = \exp(2i\delta_{l-}) = \exp(2i\delta_l) \quad (18.249)$$

since the functions  $u_{l\pm}$  satisfy the same equation in this case. Hence the amplitude  $g$  vanishes and eq. (18.243) reduces to the familiar form (4.63), namely

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)[\exp(2i\delta_l) - 1] P_l(\cos \theta).$$

### 18.3.3. Polarization phenomena in spin 0-spin $\frac{1}{2}$ scattering

Let us return to the expression (18.117) giving the differential cross section in terms of the  $M$  matrix. For spin 0-spin  $\frac{1}{2}$  scattering the differential scattering cross section for a transition  $(\mathbf{k}_i, v \rightarrow \mathbf{k}_f, v')$  is given by eq. (18.236), namely

$$\frac{d\sigma}{d\Omega}(v \rightarrow v') = |\langle v' | M | v \rangle|^2 \quad (18.250)$$

or, more explicitly

$$\frac{d\sigma}{d\Omega}(v \rightarrow v') = |\langle \chi_{v'} | f + \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} g | \chi_v \rangle|^2 \quad (18.251)$$

where we have used eq. (18.221) and denoted the initial and final spin  $\frac{1}{2}$  eigenvectors by  $\chi_v$  and  $\chi_{v'}$ , respectively. If we do not measure the spin orientations in the final state, the differential cross section for elastic scattering (from a given initial spin orientation  $v$ ) is

$$\frac{d\sigma_v}{d\Omega} = \sum_{v'} |\langle \chi_{v'} | M | \chi_v \rangle|^2 \quad (18.252)$$

or

$$\frac{d\sigma_v}{d\Omega} = |\langle \chi_v | M^\dagger M | \chi_v \rangle|^2 \quad (18.253)$$

so that

$$\frac{d\sigma_v}{d\Omega} = |f|^2 + |g|^2 + \langle \chi_v | \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} (f^*g + fg^*) | \chi_v \rangle. \quad (18.254)$$

Let us introduce the *initial polarization vector* [see eq. (15.132)]

$$\mathbf{P}_i = \langle \chi_v | \boldsymbol{\sigma} | \chi_v \rangle. \quad (18.255)$$

According to the discussion of Section 15.5.2 we remark that if the system is initially in a *pure spin state* described by the spinor  $\chi_v$ , we have  $|\mathbf{P}_i| = 1$ . Furthermore, if  $\chi_\uparrow$  and  $\chi_\downarrow$  are respectively the spin wave functions corresponding to spin “up” and spin “down”, with  $\mathbf{P}_i$  chosen as the quantization axis, we note from eqs. (15.137) that in this case

$$\boldsymbol{\sigma} \cdot \mathbf{P}_i | \chi_\uparrow \rangle = | \chi_\uparrow \rangle, \quad \boldsymbol{\sigma} \cdot \mathbf{P}_i | \chi_\downarrow \rangle = - | \chi_\downarrow \rangle. \quad (18.256)$$

Using eq. (18.255) we may write the differential cross section (18.254) as

$$\frac{d\sigma_v}{d\Omega} = |f|^2 + |g|^2 + (f^*g + fg^*) \hat{\mathbf{n}} \cdot \mathbf{P}_i \quad (18.257)$$

and we see that in general the differential cross section  $d\sigma_v/d\Omega$  depends not only on  $k$  and  $\theta$ , but also on the spin orientation of the incident particles (more exactly, on the angle between the normal  $\hat{\mathbf{n}}$  to the scattering plane and the direction of polarization  $\mathbf{P}_i$ ). The only exception occurs when

$$f^*g + fg^* = 0$$

i.e. when  $\text{Re}(fg^*) = 0$ . Since the "spin-flip" amplitude  $g$ , as given by eq. (18.248), is proportional to  $\sin \theta$ , we see that  $d\sigma_v/d\Omega$  will in general exhibit a *left-right asymmetry* [except, of course, when  $\text{Re}(fg^*) = 0$ ].

If the system is *completely unpolarized* in the initial state (i.e. composed of an equal and incoherent mixture of states  $\chi_{v=1/2}$  and  $\chi_{v=-1/2}$ ), we have  $P_i = 0$ . We note that if we average the expression (18.257) over the initial spin orientations, and call  $d\bar{\sigma}/d\Omega$  the corresponding cross section, we have

$$\frac{d\bar{\sigma}}{d\Omega} = \left( \frac{d\sigma}{d\Omega} \right)_{\text{unpol}} = |f|^2 + |g|^2 \quad (18.258)$$

where  $(d\sigma/d\Omega)_{\text{unpol}}$  is the differential cross section for a completely unpolarized initial system.

We now illustrate eq. (18.257) on two simple examples. We first choose the axis of quantization along the vector  $\hat{n}$  perpendicular to the scattering plane. If we denote by  $\chi_{v=1/2}$  and  $\chi_{v=-1/2}$  the spinors which describe incident particles respectively polarized parallel or antiparallel to  $\hat{n}$ , we find from eq. (18.255) that

$$\hat{n} \cdot \mathbf{P}_i = +1, \quad v = \frac{1}{2}$$

and

$$\hat{n} \cdot \mathbf{P}_i = -1, \quad v = -\frac{1}{2} \quad (18.259)$$

so that

$$\frac{d\sigma_{\pm 1/2}}{d\Omega} = |f|^2 + |g|^2 \pm (f^*g + fg^*). \quad (18.260)$$

We see that in this case the  $2 \times 2$  matrix  $M$  has the simple structure

$$\langle v' | M | v \rangle = \delta_{v',v} [f \pm g], \quad v' = \pm \frac{1}{2} \quad (18.261)$$

so that no spin-flip is allowed. More explicitly,

$$(M) = \begin{pmatrix} \langle \frac{1}{2} | M | \frac{1}{2} \rangle & \langle \frac{1}{2} | M | -\frac{1}{2} \rangle \\ \langle -\frac{1}{2} | M | \frac{1}{2} \rangle & \langle -\frac{1}{2} | M | -\frac{1}{2} \rangle \end{pmatrix} = \begin{pmatrix} f + g & 0 \\ 0 & f - g \end{pmatrix} \quad (18.262)$$

and eq. (18.252) reduces to

$$\frac{d\sigma_{\pm 1/2}}{d\Omega} = |\langle \pm \frac{1}{2} | M | \pm \frac{1}{2} \rangle|^2 = |\langle \pm \frac{1}{2} | f \pm g | \pm \frac{1}{2} \rangle|^2 = |f \pm g|^2 \quad (18.263)$$

which is precisely eq. (18.260).

Another interesting particular case is obtained by choosing the  $z$ -axis along  $\mathbf{k}_i$ , with the  $x$ -axis parallel to  $\hat{n}$ . We have then

$$M = f + \sigma_x g \quad (18.264)$$

or, by using the explicit form of the Pauli matrix  $\sigma_x$  given in eq. (18.216)

$$(M) = \begin{pmatrix} f & g \\ g & f \end{pmatrix}. \quad (18.265)$$

Hence the differential cross section for scattering without spin-flip is given by

$$\frac{d\sigma}{d\Omega}(\uparrow \rightarrow \uparrow) = \frac{d\sigma}{d\Omega}(\downarrow \rightarrow \downarrow) = |f|^2 \quad (18.266)$$

while the spin-flip differential cross section is simply

$$\frac{d\sigma}{d\Omega}(\uparrow \rightarrow \downarrow) = \frac{d\sigma}{d\Omega}(\downarrow \rightarrow \uparrow) = |g|^2. \quad (18.267)$$

We note that in this case the cross sections (18.266) and (18.267) do not exhibit a left-right asymmetry. We also remark that if we had chosen the  $z$ -axis parallel to  $\mathbf{k}_i$ , and the  $y$ -axis along  $\hat{\mathbf{n}}$ , we would have obtained the result

$$(M) = \begin{pmatrix} f & -ig \\ ig & f \end{pmatrix} \quad (18.268)$$

leading to the same cross sections (18.266) and (18.267).

We have so far considered the polarization vector  $\mathbf{P}_i$  of the particles in the initial state. We now express the polarization of the particles scattered in the direction  $\hat{\mathbf{k}}_f$  in terms of the polarization vector

$$\mathbf{P}_f = \frac{\langle M\chi_v | \boldsymbol{\sigma} | M\chi_v \rangle}{\langle M\chi_v | M\chi_v \rangle} = \frac{\langle \chi_v | M^\dagger \boldsymbol{\sigma} M | \chi_v \rangle}{\langle \chi_v | M^\dagger M | \chi_v \rangle}. \quad (18.269)$$

Using the expression (18.221) for  $M$ , we find that

$$\mathbf{P}_f = \frac{(|f|^2 - |g|^2)\mathbf{P}_i + (fg^* + f^*g + 2|g|^2\mathbf{P}_i \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} + i(fg^* - f^*g)\mathbf{P}_i \times \hat{\mathbf{n}}}{|f|^2 + |g|^2 + (fg^* + f^*g)\hat{\mathbf{n}} \cdot \mathbf{P}_i}. \quad (18.270)$$

If the incident beam is *unpolarized*, we have  $\mathbf{P}_i = 0$ , so that the scattered beam is *polarized* along  $\hat{\mathbf{n}}$ , i.e. *perpendicular to the scattering plane*. In this case the differential cross section is given by [cf. eq. (18.258)]

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{unpol}} = |f|^2 + |g|^2 \quad (18.271)$$

and

$$\mathbf{P}_f = \frac{fg^* + f^*g}{|f|^2 + |g|^2} \hat{\mathbf{n}} = \frac{2\text{Re}(fg^*)}{|f|^2 + |g|^2} \hat{\mathbf{n}}. \quad (18.272)$$

To understand physically why the scattering produces polarization in an initially unpolarized beam, let us examine the *classical trajectories* of spin  $\frac{1}{2}$  particles scattered by very massive spin zero particles. We therefore suppose that the interaction potential varies slowly over a de Broglie wavelength of the incident particle, so that we may use a *semi-classical model* in which the classical trajectories of the spin  $\frac{1}{2}$  particles have a meaning. Let us choose the axis of quantization to be along  $\hat{\mathbf{n}}$  (i.e. perpendicular to the scattering plane) and consider a beam which is completely polarized upward in the initial state (see Fig. 18.3). The orbital angular momentum  $\mathbf{L}$  of the particles

is evidently perpendicular to the scattering plane, but its direction for particles initially incident on the left of the scattering center is opposite to that for particles whose incident trajectories lie to the right of the scattering center. Therefore the spin-orbit part of the potential (18.224) has opposite sign in the two cases, so that for a given angle of deflection the number of particles scattered to the left or to the right will be different. For example, if we assume that  $V_c$  and  $V_s$  are both negative, but that  $|V_s| \ll |V_c|$ , then the full interaction  $V$  given by eq. (18.224) will remain attractive during the scattering

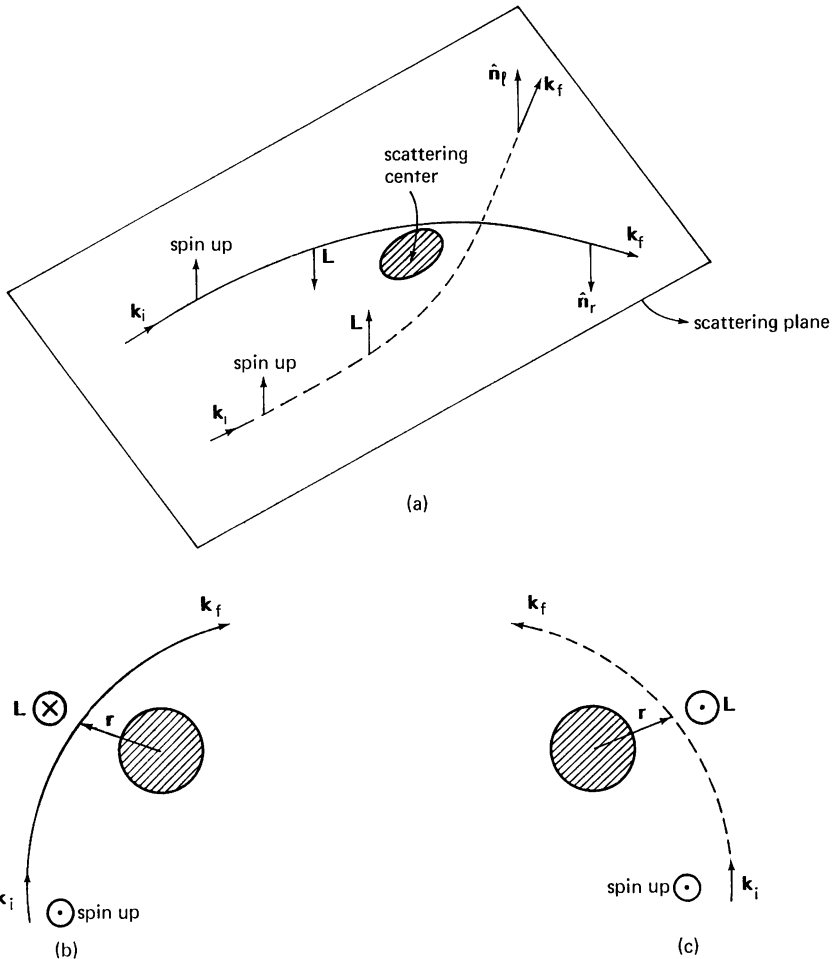


Fig. 18.3. Semi-classical illustration of the scattering of a beam initially polarized with spin up by an attractive center of force (a). General view of the scattering (b). Trajectory of particle passing to the left of the center of force (orbital angular momentum "down") and deflected to the right (c). Trajectory of particle passing to the right of the center of force (orbital angular momentum "up") and deflected to the left.

process. Hence the particles will be deflected in the way shown in Fig. 18.3 (a), i.e. to the right when they pass to the left of the scattering center and to the left when they are incident on the right of the center of force. Since the spin and angular momentum are *parallel* for particles incident to the right [see Figs. 18.3 (a) and (c)] the interaction  $V$  is strongly attractive in that case and more particles will be deflected to the left than to the right. Of course, if the initial particles were polarized with spin-down in the initial state, more particles would be deflected to the right than to the left (for the type of attractive potential which we have chosen in this example). This is the origin of the *left-right asymmetry* noted in connection with eq. (18.257). Since an incident *unpolarized* beam can be considered as a superposition of spin-up and spin-down beams of equal intensities, the total number of particles scattered to the left and right will be the same when the initial beam is unpolarized. The left-right asymmetry is then cancelled, and the differential cross section, given by eq. (18.258) is a function only of the scattering angle  $\theta$  and of the energy (or the wave number  $k$ ).

Let us now analyze the polarization of the outgoing particles. For an incident beam completely polarized upward in the initial state, the polarization clearly *remains up* [40], since no spin-flip is allowed with our choice of quantization axis along  $\hat{n}$ . Conversely, for an initial beam polarized with spin-down the polarization *remains down*. Now, in the example chosen more particles having initially spin-up will be scattered to the left, while more particles with initial spin-down are deflected to the right. Hence, for an initial *unpolarized beam* (i.e. a superposition of spin-up and spin-down beams of equal intensities) the beam scattered to the left will have net *upward* polarization, that scattered to the right will have net *downward* polarization. That is, if we measure the spin orientation of the particles scattered, say, to the right, we shall find that more of them have spin down than spin up. This clearly provides a way of obtaining *polarized beams* of particles.

Let us check that our description is consistent with the result (18.272) obtained for the polarization of the outgoing particles. Using eq. (18.263) we find that for an initial spin-up beam we have for scattering to the right ( $\hat{n}_r$  anti-parallel to  $P_i$ ),

$$\left(\frac{d\sigma_{\text{up}}}{d\Omega}\right)_{\text{right}} = |f - g|^2 \quad (18.273a)$$

while for scattering to the left ( $\hat{n}_l$  parallel to  $P_i$ )

$$\left(\frac{d\sigma_{\text{up}}}{d\Omega}\right)_{\text{left}} = |f + g|^2. \quad (18.273b)$$

Conversely, for an initial spin-down beam we have for scattering to the right ( $\hat{n}_r$  parallel to  $P_i$ )

$$\left(\frac{d\sigma_{\text{down}}}{d\Omega}\right)_{\text{right}} = |f + g|^2 \quad (18.273c)$$

while for scattering to the left ( $\hat{n}_l$  anti-parallel to  $P_l$ )

$$\left(\frac{d\sigma_{\text{down}}}{d\Omega}\right)_{\text{left}} = |f - g|^2. \quad (18.273d)$$

Hence, for an unpolarized beam

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{unpol}} = \frac{1}{2} \left( \frac{d\sigma_{\text{up}}}{d\Omega} + \frac{d\sigma_{\text{down}}}{d\Omega} \right) = |f|^2 + |g|^2$$

and

$$P_r = \frac{1}{2} \frac{|f + g|^2 - |f - g|^2}{|f|^2 + |g|^2} \hat{n}_r = \frac{fg^* + f^*g}{|f|^2 + |g|^2} \hat{n}_r \quad (18.274a)$$

while

$$P_l = \frac{1}{2} \frac{|f + g|^2 - |f - g|^2}{|f|^2 + |g|^2} \hat{n}_l = \frac{fg^* + f^*g}{|f|^2 + |g|^2} \hat{n}_l \quad (18.274b)$$

in accordance with eqs. (18.271) and (18.272).

Finally, let us consider the question of *detecting the polarization*. One possibility is to take advantage of the fact that the differential cross section for an initially polarized beam depends in general on the angle between the normal  $\hat{n}$  and the direction of polarization  $P_l$  [cf. eq. (18.257)]. This suggests a determination of polarizations by *double scattering experiments*.

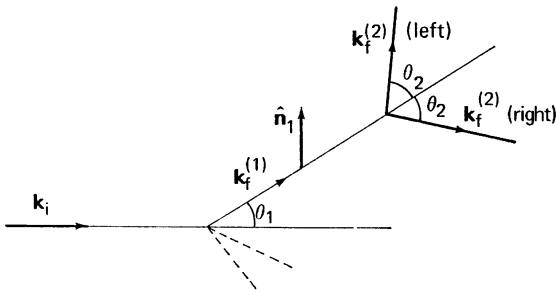


Fig. 18.4. A double scattering experiment.

Suppose, for example, that an initially unpolarized beam undergoes two successive scatterings. The differential cross section for this process may be obtained from eq. (18.254) by making in it the substitution

$$|\chi_v\rangle \rightarrow \frac{|M\chi_v\rangle}{\sqrt{\langle\chi_v|M^\dagger M|\chi_v\rangle}} \quad (18.275)$$

where the denominator accounts for the normalization of the new initial state  $|M\chi_v\rangle$ . Let us assume that the first scattering occurs through an angle  $\theta_1$  and the second scattering through an angle  $\theta_2$  (see Fig. 18.4). Furthermore, let  $k_i$ ,  $k_f^{(1)}$  and  $k_f^{(2)}$  be the respective wave vectors prior to the first scattering,

following the first scattering and after the second scattering. Let us also denote by  $\hat{n}_1$  and  $\hat{n}_2$  the normals to the first and second scattering planes, respectively, so that

$$\hat{n}_1 = \frac{\mathbf{k}_i \times \mathbf{k}_f^{(1)}}{|\mathbf{k}_i \times \mathbf{k}_f^{(1)}|}; \quad \hat{n}_2 = \frac{\mathbf{k}_f^{(1)} \times \mathbf{k}_f^{(2)}}{|\mathbf{k}_f^{(1)} \times \mathbf{k}_f^{(2)}|}. \quad (18.276)$$

Then, if  $P_1$  and  $P_2$  are the polarizations which would be obtained from the single scattering of an unpolarized beam through the angles  $\theta_1$  and  $\theta_2$ , one has

$$\frac{d\bar{\sigma}_2}{d\Omega_2} = [|f(\theta_2)|^2 + |g(\theta_2)|^2][1 + P_2(\theta_2)P_1(\theta_1)\hat{n}_1 \cdot \hat{n}_2] \quad (18.277)$$

which shows that the differential cross section  $d\bar{\sigma}_2/d\Omega_2$  depends on the angles  $\theta_1$  and  $\theta_2$ , on the magnitude of the polarizations  $P_1(\theta_1)$  and  $P_2(\theta_2)$ , and also on the angle between the two scattering planes.

If the two scatterings occur *in the same plane*, we have  $\hat{n}_1 \cdot \hat{n}_2 = +1$  or  $-1$  depending on the fact that the second scattering will occur to the left or to the right of an observer standing parallel to  $\hat{n}_1$  (see Fig. 18.4). The differential cross sections measured in the directions  $\mathbf{k}_f^{(2)}$  (left) and  $\mathbf{k}_f^{(2)}$  (right) of Fig. 18.4 will be called respectively  $(d\sigma_2/d\Omega_2)_{\text{left}}$  and  $(d\sigma_2/d\Omega_2)_{\text{right}}$ . Then

$$\frac{(d\sigma_2/d\Omega_2)_{\text{left}} - (d\sigma_2/d\Omega_2)_{\text{right}}}{(d\sigma_2/d\Omega_2)_{\text{left}} + (d\sigma_2/d\Omega_2)_{\text{right}}} = P_2(\theta_2)P_1(\theta_1). \quad (18.278)$$

The quantity

$$e = P_2(\theta_2)P_1(\theta_1) \quad (18.279)$$

is called the *asymmetry parameter*. We note from eq. (18.278) that it can be obtained from the knowledge of  $(d\sigma_2/d\Omega_2)_{\text{left}}$  and  $(d\sigma_2/d\Omega_2)_{\text{right}}$ . In order to obtain for example  $P_1$  (assuming that  $P_2$  is also unknown), we must choose the experimental setting so that the two scatterings be equivalent. That is, in the first step one scatters an unpolarized beam off a target – which acts as a polarizer – through an angle  $\theta_1$ . Then the scattered beam is scattered a second time from an *identical* target in the *same plane* through the *same* angle  $\theta_2 = \theta_1$ . Hence  $P_2(\theta_2) = P_1(\theta_1)$  and from eq. (18.279) we deduce that

$$P_1(\theta_1) = e^{1/2}. \quad (18.280)$$

So far we have considered initial systems which were completely unpolarized or else completely polarized. For initial beams (or targets) which are *partially* polarized it is convenient to use the general *density matrix formalism* of Section 15.5 [41]. Thus, from eq. (15.131) we obtain directly the initial density matrix  $\rho_i$  as

$$\rho_i = \frac{1}{2}(I + \boldsymbol{\sigma} \cdot \mathbf{P}_i) \quad (18.281)$$

where the average polarization of the incident beam is given by the polarization vector

$$\mathbf{P}_i = \text{Tr}(\rho_i \boldsymbol{\sigma}). \quad (18.282)$$



Then, substituting eqs. (18.221) and (18.281) into the expression (15.154) (valid for any degree of polarization  $0 \leq |\mathbf{P}_i| \leq 1$  of the initial system), we find that the differential cross section corresponding to the incident polarization vector  $\mathbf{P}_i$  is given by

$$\frac{d\sigma(\mathbf{P}_i)}{d\Omega} = |f|^2 + |g|^2 + (f^*g + fg^*) \hat{\mathbf{n}} \cdot \mathbf{P}_i. \quad (18.283)$$

We note that this result has exactly the form of eq. (18.257), but it is more general since we may now have  $0 \leq |\mathbf{P}_i| \leq 1$ .

We may also use the density matrix formalism to obtain the polarization  $\mathbf{P}_f$  of the scattered beam. Writing

$$\mathbf{P}_f = \text{Tr}(\rho_f \boldsymbol{\sigma}) \quad (18.284)$$

and using eq. (15.156), we have

$$\mathbf{P}_f = \frac{\text{Tr}(M \rho_i M^\dagger \boldsymbol{\sigma})}{\text{Tr}(M \rho_i M^\dagger)}. \quad (18.285)$$

For example, if the system is initially unpolarized, so that  $|\mathbf{P}_i| = 0$ , we have  $\rho_i = \frac{1}{2}I$  and

$$\begin{aligned} \text{Tr}(M \rho_i M^\dagger \boldsymbol{\sigma}) &= \frac{1}{2} \text{Tr}[(f + \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} g)(f^* + \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} g^*) \boldsymbol{\sigma}] \\ &= \frac{1}{2} (fg^* + f^*g) \text{Tr}[(\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}) \cdot \boldsymbol{\sigma}] \\ &= (fg^* + f^*g) \hat{\mathbf{n}} \end{aligned} \quad (18.286)$$

where we have used eq. (18.221) together with the fact that  $\text{Tr} \sigma_i = 0$  and  $\text{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$ . Moreover, we also have in this case

$$\text{Tr}(M \rho_i M^\dagger) = \frac{1}{2} \text{Tr}(MM^\dagger) = |f|^2 + |g|^2. \quad (18.287)$$

Therefore, using eqs. (18.286) and (18.287), we deduce from eq. (18.285) that

$$\mathbf{P}_f = \frac{2 \text{Re}(fg^*)}{|f|^2 + |g|^2} \hat{\mathbf{n}} \quad (18.288)$$

in agreement with our previous result (18.272).

Finally, we remark that polarization phenomena are also conveniently discussed by using the helicity formalism of Jacob and Wick [8].

#### 18.3.4. Total cross sections

We now write the expressions of the total cross sections for spin  $\frac{1}{2}$ -spin zero scattering. Since the elastic differential cross section averaged over the initial spin orientations is given by eq. (18.258), the total elastic cross section is simply

$$\sigma_{\text{tot}}^{\text{el}} = \int [ |f|^2 + |g|^2 ] d\Omega. \quad (18.289)$$

Using the partial wave expansions (18.243) and (18.244), together with the orthogonality of the Legendre polynomials, we have (for real or complex potentials  $V_c$  and  $V_s$ )

$$\sigma_{\text{tot}}^{\text{el}} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} \{ |(l+1)[\exp(2i\delta_{l+}) - 1] + l[\exp(2i\delta_{l-}) - 1]|^2 + l(l+1)|\exp(2i\delta_{l+}) - \exp(2i\delta_{l-})|^2 \} / (2l+1). \quad (18.290)$$

We may write this equation as

$$\sigma_{\text{tot}}^{\text{el}} = \sum_{l=0}^{\infty} \sigma_l^{\text{el}} \quad (18.291)$$

where  $\sigma_l^{\text{el}}$ , the elastic scattering cross section for the  $l$ th partial wave, is given by

$$\begin{aligned} \sigma_l^{\text{el}} &= \frac{\pi}{k^2} [(l+1)|\exp(2i\delta_{l+}) - 1|^2 + l|\exp(2i\delta_{l-}) - 1|^2] \\ &\leq 4\pi(2l+1)/k^2. \end{aligned} \quad (18.292)$$

When the potentials  $V_c$  and (or)  $V_s$  are complex (and therefore also the phase shifts  $\delta_{l\pm}$ ), we may also calculate the total cross section for removal of the incident particles from the elastic channel, i.e. the total "reaction" cross section  $\sigma_{\text{tot}}^{\text{r}}$ . A simple generalization of the partial wave method, similar to that used in Section 4.6 for scattering by spinless particles, yields

$$\sigma_{\text{tot}}^{\text{r}} = \sum_{l=0}^{\infty} \sigma_l^{\text{r}} \quad (18.293)$$

where

$$\begin{aligned} \sigma_l^{\text{r}} &= \frac{\pi}{k^2} [(2l+1) - (l+1)|\exp(2i\delta_{l+})|^2 - l|\exp(2i\delta_{l-})|^2] \\ &\leq \pi(2l+1)/k^2. \end{aligned} \quad (18.294)$$

If only *elastic* scattering occurs, so that the phase shifts  $\delta_{l\pm}$  are real, we have evidently  $\sigma_{\text{tot}}^{\text{r}} = 0$  and

$$\sigma_l^{\text{el}} = \frac{4\pi}{k^2} [(l+1) \sin^2 \delta_{l+} + l \sin^2 \delta_{l-}] \leq 4\pi(2l+1)/k^2. \quad (18.295)$$

Finally, for spinless particles, or in the absence of spin-orbit forces, the results (18.290)–(18.295) evidently reduce to the familiar formulae which we derived in Section 4.1 [eqs. (4.71)–(4.72)] for real potentials and in Section 4.6 [eqs. (4.260)–(4.261) and (4.268)–(4.272)] for complex potentials.

### 18.4. Hadronic collisions at high energies

In this section we want to indicate how the Regge pole ideas introduced in Chapter 11 in the framework of potential scattering may be used to describe two-body hadronic collisions at high energies. We shall only give here a simple, introductory account of this subject which has received a considerable amount of attention during the recent years. A few important references are given at the end of this chapter [42–56].

First of all, let us stress that the point of view which we shall adopt in analyzing the high-energy Regge pole model is very different from our study of Regge poles in Section 11.4. In potential scattering the existence of Regge poles and their properties are a consequence of the mathematical properties of the Schrödinger equation which governs the dynamics of the problem. On the contrary, in high-energy, strong interaction physics there does not exist at present a well-established dynamical framework. The general principles of relativistic invariance, unitarity and crossing symmetry, although very powerful, do not seem to constitute a complete dynamics. As a consequence, the Regge pole model for strong interactions has not been “derived” from first principles, and is therefore a phenomenological theory in which one attempts to obtain agreement with experiment in the most economical way, i.e. by using the smallest possible number of free parameters.

With these ideas in mind, let us consider the following very simple model. We conjecture that the results which may be taken over from the potential scattering approach to hadronic interactions are:

1) The partial wave amplitudes  $a(l, E)$  can be defined for complex  $l$ -values. They are analytic for  $\text{Re } l > -\frac{1}{2}$ , except for a finite number of isolated Regge poles of order one.

2) When  $|l| \rightarrow \infty$ , the quantity  $|a(l, E)|$  behaves in such a way that there is no contribution from the circle at infinity to the Regge–Sommerfeld–Watson transform.

We recall that these assumptions, together with the notion of signature introduced in Section 11.4 in connection with *exchange forces* imply the RSW representation of the scattering amplitude [see eq. (11.158)], namely,

$$f(E, \cos \theta) = \sum_i \frac{\beta_i(E)}{\sin \pi \alpha_i(E)} \{ P_{\alpha_i(E)}(-\cos \theta) + \tau_i P_{\alpha_i(E)}(\cos \theta) \} + BI(E, \cos \theta) \quad (18.296)$$

where we have written the background integral as BI instead of  $\tilde{BI}$ . The quantities  $\tau_i$  are the signatures of the Regge poles. That is,  $\tau_i = +1$  for a Regge pole of  $a^+(l, E)$  and  $\tau_i = -1$  for a Regge pole of  $a^-(l, E)$ . We also deduce from these assumptions that a Regge pole gives bound states and resonances in the way described in Section 11.4.

The implications of these ideas in hadron physics are the following:

1) Regge trajectories relate particles with the same internal quantum numbers (baryon number, isospin, strangeness, etc.) but different spins.

2) Regge trajectories govern the high-energy (asymptotic) behaviour of two-body hadronic reactions.

Let us first consider the first point. With the assumptions made above Regge trajectories will pass through bound states and resonances as in the case of potential scattering. Because of exchange forces and the signature concept, a Regge pole will only appear as a particle or a resonance at values of  $l$  (or  $J$ , the spin of the particle) which differ by two units. Furthermore, we must also take into account the fact that a scattering amplitude is now labelled by various internal quantum numbers such as baryon number, isospin, etc. Hence, *the Regge trajectories of hadron physics relate particles with the same internal quantum numbers but different spins which differ by two units.* It is customary to plot these trajectories in the so-called *Chew–Frautschi diagram* [spin  $J$  versus the square of the mass  $m^2$  of the particles, expressed in  $(\text{GeV})^2$ ] where they appear experimentally to lie on straight lines. An example of such Regge trajectories is given in Fig. 18.5 for the case of the nucleon resonances  $\Delta$ , with isospin  $I = \frac{3}{2}$  and hypercharge  $Y = +1$ . It is worth noting that instead of associating Regge trajectories with scattering amplitudes, we may also consider them to be simply characterized by sets of quantum numbers, just like particles. Such “particles”, whose mass depend on their spin are called *Reggeons*.

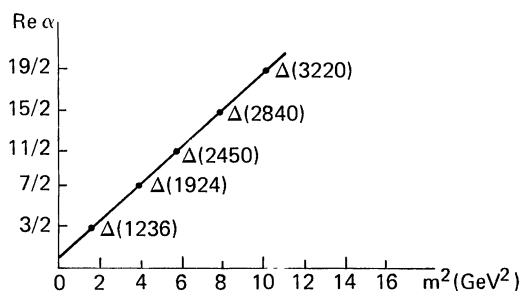


Fig. 18.5. Regge recurrences for the nucleon resonances ( $I = \frac{3}{2}$ ,  $Y = +1$ ).

We now examine how Regge trajectories may be used to study the high-energy behaviour of two-body hadronic collisions. The key concept which we shall use for this purpose is the principle of *crossing symmetry*.

Let us consider a two-body reaction in the  $s$ -channel [see Section 2.2]



This reaction is illustrated in Fig. 18.6, together with the associated four-momenta  $p_A$ ,  $p_B$ ,  $p_C$  and  $p_D$ . We consider also the corresponding  $t$ -channel and  $u$ -channel reactions, namely



and

$$A + \bar{D} \rightarrow \bar{B} + C \quad (u \text{ channel}). \quad (18.299)$$

The  $t$ -channel reaction (18.298) is also illustrated on Fig. 18.6.

In what follows, we shall neglect the spins of the particles, so that to each of the three reactions there corresponds *one* (relativistic) amplitude. We denote these amplitudes respectively by  $A_s$ ,  $A_t$ ,  $A_u$ . While a priori there could be no relation between the amplitudes  $A_s$ ,  $A_t$  and  $A_u$ , the principle of crossing symmetry tells us that the following *substitution rule* applies:

$$A_t(p_A, p_C, p_B, p_D) = A_s(p_A, p_B = -p_B, p_C = -p_C, p_D) \quad (18.300a)$$

and

$$A_u(p_A, p_{\bar{D}}, p_B, p_C) = A_s(p_A, p_B = -p_B, p_C, p_D = -p_D). \quad (18.300b)$$

In terms of the Mandelstam variables, we then have for example

$$A_t(s, t) = A_s(s = (p_A - p_B)^2, t = (p_A + p_C)^2) \quad (18.301a)$$

and

$$A_u(s, u) = A_s(s = (p_A - p_B)^2, u = (p_A + p_D)^2). \quad (18.301b)$$

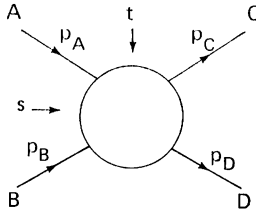


Fig. 18.6. The  $s$ - and  $t$ -channel reactions (18.297) and (18.298).

We recall that in going from the  $s$  channel to the  $t$  channel the energy variable  $s$  becomes a momentum transfer variable while the momentum transfer variable  $t$  now represents the square of the C.M. energy in the  $t$  channel. Similarly, in going from the  $s$  to the  $u$  channel the energy variable  $s$  becomes a momentum transfer variable, while the momentum transfer variable  $u$  now corresponds to the C.M. energy squared in the  $u$  channel. Thus the crossing relations (18.301) imply that the  $t$ -channel and  $u$ -channel amplitudes  $A_t$  and  $A_u$  are given by the *same analytic expression* which gives  $A_s$ , but for *different values of the variables*. In other words, the same analytic function  $A(s, t, u)$  represents the three scattering amplitudes  $A_s$ ,  $A_t$  and  $A_u$ . In the physical region of the  $s$ -channel reaction (18.297), the value of this function gives the physical scattering amplitude for this reaction. The same is true for the  $t$  and  $u$  channels.

Since the physical regions of the  $s$ -,  $t$ - and  $u$ -channel reactions do not overlap (cf. the Mandelstam diagram and the discussion of physical regions in Section 2.2), it is by *analytic continuation* [57] from one physical region to the other that the amplitudes  $A_s$ ,  $A_t$  and  $A_u$  are connected.

Having recalled the basic concept of crossing symmetry, we are now prepared to extract the asymptotic behaviour of high-energy two-body hadronic collisions (within the context of the simple Regge pole model considered here). To this end, we first examine the reaction (18.298) in the  $t$ -channel and apply to it the RSW representation, neglecting for the moment the signature. We consider the  $t$ -channel amplitude  $A_t(s, t)$  and write [58]

$$A_t(s, t) = \sum_i \frac{\beta_i(t)}{\sin \pi \alpha_i(t)} P_{\alpha_i(t)}(-\cos \theta_t) + \text{BI}(t, \cos \theta_t) \quad (18.302)$$

where  $t$  is the square of the C.M. energy in the  $t$  channel and  $\cos \theta_t$  depends on  $s$  and  $t$ .

We now invoke crossing symmetry to infer that the  $s$ -channel amplitude  $A_s(s, t)$  is given by the same expression, in which  $\cos \theta_t$  is expressed in terms of  $s$  and  $t$ . For the simple case of a reaction such that  $m_A = m_C = m$  and  $m_B = m_D = M$ , we have from eq. (2.122),

$$\cos \theta_t = \frac{2[s + \frac{1}{2}t - m^2 - M^2]}{\sqrt{t - 4m^2}\sqrt{t - 4M^2}} \simeq \frac{-2s}{\sqrt{4m^2 - t}\sqrt{4M^2 - t}} \sim (-s). \quad (18.303)$$

Here we have considered the *high energy limit in the  $s$  channel* (for fixed  $t$ ) and have therefore neglected the quantities  $m^2$ ,  $M^2$  and  $t$  by comparison with  $s$ . We have also extracted a factor (i) from each square root in order to obtain square roots of positive quantities in the  $s$  channel. We remark at this point that  $|\cos \theta_t|$  becomes very large when  $s$  increases, but this should be no cause for alarm since the quantity  $\theta_t$  is only the scattering angle in the  $t$  channel *physical region*, and we are now in the *physical region* of the  $s$  channel. Because for  $\alpha$  complex such that  $\text{Re } \alpha > -\frac{1}{2}$  one has

$$P_\alpha(x) \underset{x \rightarrow \pm \infty}{\sim} C(\alpha)x^\alpha; \quad C(\alpha) = \frac{2^\alpha \Gamma(\alpha + \frac{1}{2})}{\pi^{1/2} \Gamma(\alpha + 1)} \quad (18.304)$$

we may write, for high energies in the  $s$  channel

$$A_s(s, t) = \sum_i \frac{\tilde{\beta}_i(t)}{\sin \pi \alpha_i(t)} \left\{ \frac{s}{s_0} \right\}^{\alpha_i(t)} + \text{BI} \quad (18.305)$$

where the function  $\tilde{\beta}_i(t)$  contains all  $s$ -independent quantities. The scale factor  $s_0$  is introduced here for convenience; it has the same dimensions as  $s$ , so that the power of a dimensionless number appears in eq. (18.305). Since the background integral may be shown to be proportional to  $s^{-1/2}$ , it follows that when exchange forces are neglected,

$$A_s(s, t) \xrightarrow{s \rightarrow \infty} \sum_i \frac{\tilde{\beta}_i(t)}{\sin \pi \alpha_i(t)} \left\{ \frac{s}{s_0} \right\}^{\alpha_i(t)} + \mathcal{O}(s^{-1/2}). \quad (18.306)$$

Let us now take into account the signature of the Regge poles. A detailed analysis of the analytic continuation from the  $t$  channel to the  $s$  channel shows that eq. (18.306) must be replaced in this case by

$$A_s(s, t) \rightarrow \sum_{i \text{ fixed}} \gamma_i^\pm(t) \xi_i^\pm(t) \left\{ \frac{s}{s_0} \right\}^{\alpha_i^\pm(t)} \quad (18.307)$$

where the quantities  $\gamma_i^\pm(t)$  are called the *residue functions*, and the *signature factors*  $\xi_i^\pm(t)$  are given by [53]

$$\xi_i^\pm(t) = \frac{1 + \tau_i \exp\{-i\pi\alpha_i^\pm(t)\}}{\sin \pi \alpha_i^\pm(t)}, \quad \tau_i = \pm 1. \quad (18.308)$$

Therefore, the RSW representation, initially written down in terms of Regge trajectories  $\alpha_i(t)$  in the  $t$  channel, allows us by invoking crossing symmetry to make predictions about the asymptotic behaviour of the scattering amplitude in the  $s$  channel *physical region* ( $s \rightarrow \infty$ ,  $t$  fixed and negative). The Regge trajectories  $\alpha_i^\pm(t)$ , continued in the  $s$  channel are called the *exchanged* Regge trajectories in the  $s$  channel. If we order the Regge trajectories in such a way that

$$\operatorname{Re} \alpha_1^\pm \geq \operatorname{Re} \alpha_2^\pm \geq \dots \geq -\frac{1}{2} \quad (18.309)$$

we may write eq. (18.307) as

$$A_s(s, t) \rightarrow \gamma_1^\pm(t) \xi_1^\pm(t) \left( \frac{s}{s_0} \right)^{\alpha_1^\pm(t)} + \gamma_2^\pm(t) \xi_2^\pm(t) \left( \frac{s}{s_0} \right)^{\alpha_2^\pm(t)} + \dots \quad (18.310)$$

which is simply a representation of the  $s$  channel scattering amplitude as a descending asymptotic series in powers of the variable  $s$ .

A simple physical picture of the trajectories “exchanged” in an  $s$  channel reaction may be given, as shown by the diagram of Fig. 18.7. In this case we say that the two particles A and B colliding in the  $s$  channel have exchanged a Reggeon. This exchange is therefore similar to a (Yukawa) force which acts between the two particles. On the contrary, in the  $t$  channel (see Fig. 18.7), the Reggeon appears as an “intermediate state” of the particles A and  $\bar{C}$  (or  $\bar{B}$  and D) which accounts for bound states and resonances in that channel. Hence, in the Regge model, forces arise from the exchange of Reggeons that can act as “intermediate states” for crossed reactions.

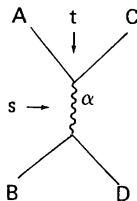


Fig. 18.7. Exchange of a Reggeon in the reaction  $A + B \rightarrow C + D$ .

So far we have considered the crossing from the  $t$  channel to the  $s$  channel. Similarly, by crossing from the  $u$  channel to the  $s$  channel, we obtain

$$A_s(s, u) \rightarrow \sum_{\substack{s \rightarrow \infty \\ u \text{ fixed}}} \gamma_j^\pm(u) \xi_j^\pm(u) \left\{ \frac{s}{s_0} \right\}^{\alpha_j^\pm(u)} \quad (18.311)$$

where  $\alpha_j^\pm(u)$  are the signed Regge trajectories of the  $u$  channel, continued into the  $s$  channel. Since the  $u$  and  $t$  channels may have different quantum numbers, the trajectories  $\alpha_i^\pm(t)$  and  $\alpha_j^\pm(u)$  are in general different.

To summarize, the two equations (18.307) and (18.311) give the asymptotic behaviour of the scattering amplitude in the  $s$  channel in terms of Regge trajectories in the  $t$  and  $u$  channels. These are in turn connected to the bound states and resonances in the  $t$  and  $u$  channels. It is worth noting that a Regge trajectory  $\alpha^\pm(t)$  in the  $t$  channel is only accessible to experiment when it increases through a positive integer such that the rule  $\Delta J = 2$  is obeyed. On the contrary, for  $t \leq 0$  (i.e. in the physical region of the  $s$  channel where the variable  $t$  is now the square of a four-momentum transfer), the Regge trajectory is in principle accessible for all values of  $t$ . This is illustrated in Fig. 18.8 where a typical (real) Regge trajectory is shown.

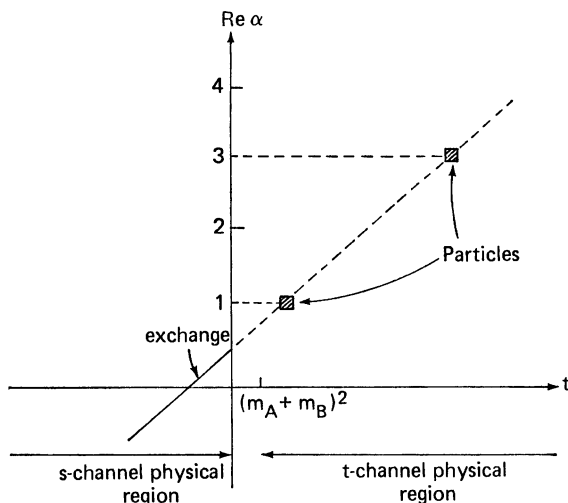


Fig. 18.8. The trajectory of an odd signature Regge pole which yields particles of spin 1 and 3 in the  $t$ -channel physical region, and is exchanged in the  $s$ -channel physical region.

We shall not discuss here the numerous applications of eqs. (18.307) and (18.311) to particular high-energy two-body reactions. We simply point out that the Regge pole theory has been very useful in the analysis of high-energy data. We note, however, that the simple model described above allows only for the presence of a finite number of isolated Regge poles of order one in



the scattering amplitudes. In fact more complicated singularities such as cuts, fixed poles, families of poles ("daughter trajectories"), etc. should be considered and various special assumptions of the simple Regge pole model must therefore be abandoned. It is probable, however, that the basic methods of complex angular momentum will remain useful to analyze high-energy hadronic collisions.

## References and notes

- [1] We recall that by "elementary" particles we mean objects which in the particular process considered do not exhibit a *composite* structure (i.e. are not bound states of other particles). Elementary particles may of course possess internal degrees of freedom such as spin, isospin, strangeness, etc.
- [2] This analysis is easily extended to include isospin modifications. General two-body reactions of the type  $A + B \rightarrow C + D$  (e.g. the associated production process  $\pi^+ + p \rightarrow K^+ + \Sigma^+$ ) where two "elementary" particles are present in the initial and final states will be taken up in Section 18.2.
- [3] A summary of the main properties of vector addition coefficients is given in Appendix E.
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- [6] The geometry of the situation is described by Fig. 4.3.
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- [20] This generalization is similar to the introduction of the *vector spherical harmonics* in electromagnetism.
- [21] GOLDBERGER, M. L. and K. M. WATSON (1964), *Collision Theory* (Wiley, New York) Chapter 7.
- [22] Of course it may happen that  $l = l'$  and  $S = S'$  in some particular cases. For example, if one of the particles has spin  $\frac{1}{2}$  and the other spin 0, the total value of  $S$  must be  $\frac{1}{2}$  and the only two possible values of  $l$  for a given  $J$  are  $l = J \pm \frac{1}{2}$ . Then, if *parity* is conserved, we shall see below that no transitions can occur between the states with  $l = J + \frac{1}{2}$  and those with  $l = J - \frac{1}{2}$ . Thus in this case  $l = l'$ .
- [23] We note that the radial functions  $R_{l'S',lS}^J$  now have *two* sets of subscripts. The first ( $l'S'$ ) corresponds to the relative probability of finding the system with those values of  $l'$  and  $S'$ . The second ( $lS$ ) refers to the orbital and spin angular momenta of the incident free wave.

- [24] See for example NEWTON, R. G. (1966), *Scattering Theory of Waves and Particles* (Mc-Graw-Hill, New York) Section 15.2.
- [25] NEWTON, R. G. (1960), *J. Math Phys.* **1**, 319.
- [26] NEWTON, R. G. (1964), *The complex j-plane* (Benjamin, New York).
- [27] Since  $k_f$  is related to  $k_i$  by energy conservation we shall simply write  $S(k_i)$  instead of  $S(k_i, k_f)$ .
- [28] We are considering here the case of two-body scattering. For two-body reactions we have of course  $\langle f n' l' S' | S^J(k_i) | i n l S \rangle$ .
- [29] A more complete treatment may be found in the original paper of JACOB and WICK [8]; see also GOLDBERGER, M. L. and K. M. WATSON, loc. cit. [21] Appendix E.
- [30] WIGNER, E. P. (1957), *Rev. Mod. Phys.* **29**, 255.
- [31] Indeed the product of two matrices corresponding to the two successive rotations  $R_{\alpha_1 \beta_1 \gamma_1}^{(1)}$  and  $R_{\alpha_2 \beta_2 \gamma_2}^{(2)}$  is easily seen to be the matrix corresponding to the rotation  $R_{\alpha \beta \gamma} \equiv R_{\alpha_2 \beta_2 \gamma_2}^{(2)} \cdot R_{\alpha_1 \beta_1 \gamma_1}^{(1)}$  namely  $D_{M' M}^J(\alpha \beta \gamma) = \sum_{M''} D_{M' M''}^J(\alpha_2 \beta_2 \gamma_2) D_{M'' M}^J(\alpha_1 \beta_1 \gamma_1)$ . This last relation is valid up to an arbitrary phase factor. If this phase is chosen equal to one we have a *vector representation*. Otherwise we have *ray-representations* [see for example HAMERMESH, M. (1962), *Group Theory* (Addison-Wesley, Reading, Mass.)].
- [32] We recall that in the Russell-Saunders notation the symbols S, P, D, F, G, etc. correspond to states with  $L = 0, 1, 2, 3, 4$ , etc.
- [33] This assumption, together with the requirement that  $H$  should be independent of  $I_z$  is called the postulate of *charge independence*.
- [34] See for example GOLDBERGER, M. L. and K. M. WATSON, loc. cit. [21].
- [35] In general, a unitary, symmetric  $n \times n$   $S$ -matrix depends on  $\frac{1}{2}n(n+1)$  real parameters. Indeed a complex  $n \times n$  matrix depends on  $2n^2$  real numbers. Now the unitarity requirement imposes  $n^2$  conditions, while the fact that  $S$  is symmetric induces  $\frac{1}{2}n(n-1)$  additional constraints. Hence there remain only  $2n^2 - n^2 - \frac{1}{2}n(n-1) = \frac{1}{2}n(n+1)$  real parameters. We may also find this result by noting that the real, orthogonal  $n \times n$  matrix  $A$  of eq. (18.190) depends on  $\frac{1}{2}n(n-1)$  real numbers. Adding the  $n$  eigenphase shifts, we find that  $S$  depends in general on  $\frac{1}{2}n(n+1)$  real parameters.
- [36] In counting the allowed states one must also remember the restriction  $J \geq |\lambda_1 - \lambda_2|$ .
- [37] In what follows we shall write either  $\sigma \equiv (\sigma_x, \sigma_y, \sigma_z)$  or  $\sigma \equiv (\sigma_1, \sigma_2, \sigma_3)$ .
- [38] The potential  $V$  given in eq. (18.224) is not the most general spin 0-spin  $\frac{1}{2}$  interaction since  $V_c$  and (or)  $V_s$  could be non-local or velocity dependent.
- [39] This situation arises when other phenomena than elastic scattering may occur (see Section 4.6). A detailed discussion of complex (optical) potentials will be made in Chapter 20.
- [40] This may of course be seen directly from eq. (18.270). Let us denote respectively by  $\hat{n}_l$  and  $\hat{n}_r$  the unit vectors  $\hat{n}$  of eq. (18.272) corresponding to a scattering to the left or to the right [see Fig. 18.3 (a)]. For particles incident to the left and scattered to the right [Fig. 18.3 (b)] we find that  $\mathbf{P}_r = -\hat{n}_r = \mathbf{P}_l$  whereas for particles incident to the right and scattered to the left [Fig. 18.3 (c)] we have  $\mathbf{P}_l = \hat{n}_l = \mathbf{P}_r$ .
- [41] See for example WOLFENSTEIN [11]; WOLFENSTEIN and ASHKIN [12]; GOLDBERGER and WATSON [21].
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- [56] PHILLIPS, R. J. N. (1972), Proc. 1972 CERN School of Physics at Grado (CERN, Geneva), p. 541.
- [57] This analytic continuation must be done in a suitable way: it must avoid the possible cuts and preserve four-momentum conservation.
- [58] The normalization of  $A(s, t)$  is such that at high energies in the  $s$  channel ( $s$  large) the optical theorem reads  $\sigma_{\text{tot}} = s^{-1} \text{Im } A_s^{\text{el}}(s, t = 0)$ . Furthermore, we discard here the variable  $u$ , since we know that the three Mandelstam variables  $s, t, u$  are not independent [see eq. (2.117)].

## Three-Body Problems

In this chapter we want to give an introduction to some of the techniques aiming at the solution of three-body problems. We first introduce in Section 19.1 some convenient definitions and notations. In Section 19.2 we return to the difficulties encountered in applying the Lippmann–Schwinger equations to three-body problems. This analysis leads to the Faddeev equations [1] which are obtained and discussed in Section 19.3 for non-relativistic three-body collisions. Three-body multiple scattering expansions are discussed in Section 19.4. Finally, in Sections 19.5 and 19.6 we analyze in detail two particularly important three-body problems: electron collisions with atomic hydrogen and high-energy hadron–deuteron scattering.

### *19.1. Definitions and notations*

Let us assume that the three particles 1, 2, 3 having masses  $m_1$ ,  $m_2$ ,  $m_3$ , interact by means of two-body potentials. We shall denote by  $V^1 \equiv V_{23}$  the potential acting between particles 2 and 3, while  $V^2 \equiv V_{13}$  acts between 1 and 3 and  $V^3 \equiv V_{12}$  between 1 and 2.

We assume for the moment that the system is non-relativistic and we write its total Hamiltonian as

$$H = H_0 + V \quad (19.1)$$

where  $H_0$  is the kinetic energy operator of the system and

$$V = \sum_{i=1}^3 V^i \quad (19.2)$$

is the total interaction potential. The Green's operators corresponding to  $H$  and  $H_0$  are respectively

$$G^{(\pm)}(E) = \frac{1}{E - H \pm i\varepsilon} \quad (19.3)$$

and

$$G_0^{(\pm)}(E) = \frac{1}{E - H_0 \pm i\varepsilon}. \quad (19.4)$$

We shall also need the Hamiltonian describing two particles interacting while the third one is free, namely

$$H_i = H_0 + V^i \quad (19.5)$$

with the corresponding Green's operators

$$G_i^{(\pm)}(E) = \frac{1}{E - H_i \pm i\varepsilon}. \quad (19.6)$$

We also define the operators

$$V_i = V - V^i \quad (19.7)$$

corresponding to the interactions in which particle  $i$  participates. For example

$$V_1 = V - V^1 = V - V_{23} = V_{12} + V_{13}.$$

Let us introduce the two-body transition operators

$$T_i = V^i + V^i G_i^{(+)} V^i \quad (19.8)$$

which satisfy the Lippmann-Schwinger equations

$$T_i = V^i + T_i G_0^{(+)} V^i \quad (19.9a)$$

and

$$T_i = V^i + V^i G_0^{(+)} T_i. \quad (19.9b)$$

We note that

$$G_i^{(\pm)} = G_0^{(\pm)} + G_0^{(\pm)} V^i G_i^{(\pm)} \quad (19.10a)$$

$$= G_0^{(\pm)} + G_i^{(\pm)} V^i G_0^{(\pm)} \quad (19.10b)$$

and

$$G_i^{(+)} = G_0^{(+)} + G_0^{(+)} T_i G_0^{(+)}. \quad (19.10c)$$

Moreover, we also see that

$$G_i^{(+)} V^i = G_0^{(+)} T_i. \quad (19.11)$$

Finally, the full three-body  $\mathcal{T}$ -operator is given by [see eq. (14.172)]

$$\mathcal{T} = V + V G^{(+)} V \quad (19.12)$$

and satisfies the Lippmann-Schwinger equations

$$\mathcal{T} = V + V G_0^{(+)} \mathcal{T} \quad (19.13a)$$

and

$$\mathcal{T} = V + \mathcal{T} G_0^{(+)} V \quad (19.13b)$$

with

$$G^{(+)}V = G_0^{(+)}\mathcal{T}. \quad (19.13c)$$

Before we analyze how these operators act in the three-body Hilbert space, let us discuss some kinematical questions. We shall denote by  $\mathbf{p}_i$  the momentum of particle  $i$ . The total momentum is then given by

$$\mathbf{P} = \sum_{i=1}^3 \mathbf{p}_i.$$

If we elect to work in the total C.M. system, the condition  $\mathbf{P} = 0$  tells us that only two of the three momenta are independent. A convenient choice consists in using the momentum of one particle  $\mathbf{p}_i$ , together with the relative momentum

$$\mathbf{q}_i = \frac{m_k \mathbf{p}_j - m_j \mathbf{p}_k}{m_j + m_k} \quad (i, j, k = 1, 2, 3) \quad (19.14)$$

of the two other particles. Here  $(i, j, k)$  form a cyclic permutation so that, for example

$$\mathbf{q}_1 = \frac{m_3 \mathbf{p}_2 - m_2 \mathbf{p}_3}{m_2 + m_3}.$$

Denoting by  $\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3$  the coordinates of the three particles with respect to a fixed origin, we note that the two momenta  $\mathbf{p}_i$  and  $\mathbf{q}_i$  are respectively the conjugate momenta of the two vectors

$$\mathbf{r}_i = \mathbf{R}_i - \frac{m_j \mathbf{R}_j + m_k \mathbf{R}_k}{m_j + m_k} \quad (19.15)$$

and

$$\mathbf{p}_i = \mathbf{R}_j - \mathbf{R}_k \quad (i, j, k = 1, 2, 3) \quad (19.16)$$

which specify the coordinates of the three particles in the C.M. system. We see that the vector  $\mathbf{p}_i$  specifies the relative position of particles  $j$  and  $k$  while the vector  $\mathbf{r}_i$  gives the position of particle  $i$  with respect to the center of mass of  $(j, k)$ . These vectors are shown in Fig. 19.1 for the case  $i = 1, j = 2, k = 3$ .

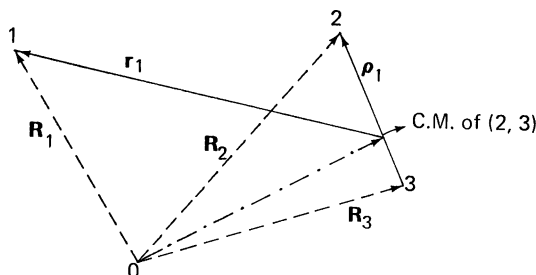


Fig. 19.1. Illustration of the vectors of the text.

In terms of the momenta  $\mathbf{P}$ ,  $\mathbf{p}_i$  and  $\mathbf{q}_i$  the kinetic energy operator is easily seen to be given by

$$H_0 = \frac{P^2}{2M} + \frac{p_i^2}{2\bar{\mu}_i} + \frac{q_i^2}{2\mu_i} \quad (19.17)$$

where

$$\begin{aligned} M &= \sum_{i=1}^3 m_i, \\ \bar{\mu}_i &= m_i(m_j + m_k)/(m_i + m_j + m_k) \\ \mu_i &= m_j m_k/(m_j + m_k). \end{aligned} \quad (19.18)$$

The physical interpretation of eq. (19.17) is straightforward. The first term is the kinetic energy of the C.M. The third term corresponds to the relative kinetic energy of particles  $j$  and  $k$  in their own C.M. system, while the second term accounts for the relative kinetic energy of particle  $i$  and the compound system  $(j, k)$ . Thus, in the C.M. system the total Hamiltonian can be written as

$$H = \frac{p_i^2}{2\bar{\mu}_i} + \frac{q_i^2}{2\mu_i} + V^1 + V^2 + V^3. \quad (19.19)$$

For example, if we have  $i = 1, j = 2, k = 3$ , we may write

$$\begin{aligned} H &= \frac{p_1^2}{2\bar{\mu}_1} + \frac{q_1^2}{2\mu_1} + V^1(\mathbf{p}_1) + V^2\left(\mathbf{r}_1 + \frac{m_2}{m_2 + m_3}\mathbf{p}_1\right) \\ &\quad + V^3\left(\mathbf{r}_1 - \frac{m_3}{m_2 + m_3}\mathbf{p}_1\right). \end{aligned} \quad (19.20)$$

To describe three-particle states, we need a three-particle Hilbert space. For example, in the momentum representation we shall write the wave function of the system as  $\Psi(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) \equiv \langle \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3 | \Psi \rangle$  and normalize the states  $|\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\rangle$  so that

$$\langle \mathbf{p}'_1, \mathbf{p}'_2, \mathbf{p}'_3 | \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3 \rangle = \delta(\mathbf{p}'_1 - \mathbf{p}_1) \delta(\mathbf{p}'_2 - \mathbf{p}_2) \delta(\mathbf{p}'_3 - \mathbf{p}_3). \quad (19.21)$$

The matrix elements of a given operator  $A$  will then be written as

$$\langle \mathbf{p}'_1, \mathbf{p}'_2, \mathbf{p}'_3 | A | \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3 \rangle. \quad (19.22)$$

In fact, since all the operators that we shall use commute with the total momentum, we may extract a momentum conserving delta function

$$\delta(\mathbf{p}'_1 + \mathbf{p}'_2 + \mathbf{p}'_3 - \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{p}_3)$$

from all the matrix elements. Hence in the C.M. system the states will be specified by two momentum variables, which we choose to be the variables  $\mathbf{p}_i$  and  $\mathbf{q}_i$  defined above. For example the two-body interaction potentials  $V^i$  have matrix elements

$$\langle \mathbf{p}'_i, \mathbf{q}'_i | V^i | \mathbf{p}_i, \mathbf{q}_i \rangle = \delta(\mathbf{p}'_i - \mathbf{p}_i) \langle \mathbf{q}'_i | V^i | \mathbf{q}_i \rangle \quad (19.23)$$

with [2]

$$\langle \mathbf{q}'_i | V^i | \mathbf{q}_i \rangle = (2\pi)^{-3} \int d\mathbf{r} \exp\{i(\mathbf{q}_i - \mathbf{q}'_i) \cdot \mathbf{r}\} V^i(\mathbf{r}). \quad (19.24)$$

Similarly

$$\langle \mathbf{p}'_i, \mathbf{q}'_i | H_0 | \mathbf{p}_i, \mathbf{q}_i \rangle = \delta(\mathbf{p}'_i - \mathbf{p}_i) \delta(\mathbf{q}'_i - \mathbf{q}_i) \left( \frac{p_i^2}{2\bar{\mu}_i} + \frac{q_i^2}{2\mu_i} \right). \quad (19.25)$$

We also need to know how to express a two-body transition matrix element in the three-body Hilbert space. Using eqs. (19.9b), (19.4), (19.23) and (19.25) we find that

$$\langle \mathbf{p}'_i, \mathbf{q}'_i | T_i(E) | \mathbf{p}_i, \mathbf{q}_i \rangle = \delta(\mathbf{p}'_i - \mathbf{p}_i) \left\langle \mathbf{q}'_i \left| T_i \left( E - \frac{p_i^2}{2\bar{\mu}_i} \right) \right| \mathbf{q}_i \right\rangle \quad (19.26)$$

with

$$\begin{aligned} \langle \mathbf{q}'_i | T_i(\xi_i) | \mathbf{q}_i \rangle &= \langle \mathbf{q}'_i | V^i | \mathbf{q}_i \rangle \\ &+ \int d\mathbf{q}''_i \langle \mathbf{q}'_i | V^i | \mathbf{q}''_i \rangle \frac{1}{\xi_i - \mathbf{q}''_i{}^2/2\mu_i + i\epsilon} \langle \mathbf{q}''_i | T_i(\xi_i) | \mathbf{q}_i \rangle \end{aligned} \quad (19.27)$$

and  $\xi_i = E - p_i^2/2\bar{\mu}_i$ . We remark that the two-body Lippmann–Schwinger equation, expressed in three-body Hilbert space, is very similar to the corresponding one written in two-body Hilbert space [see for example eq. (16.21c)] except for an overall factor  $\delta(\mathbf{p}'_i - \mathbf{p}_i)$  and a change in the energy variable.

It is convenient to introduce at this point a diagrammatic representation [3] which is quite intuitive and will help to visualize some of the key properties of three-body systems. First of all, we look at the two-body Lippmann–Schwinger equations (19.9)–(19.10). If we write the Born series expansion for  $G_i$ , namely [we suppress from now on the superscript (+)]

$$G_i = G_0 + G_0 V^i G_0 + G_0 V^i G_0 V^i G_0 + \dots$$

we obtain for  $T_i$  the perturbation expansion

$$T_i = V^i + V^i G_0 V^i + V^i G_0 V^i G_0 V^i + \dots \quad (19.28)$$

To represent this expansion, we draw a (perturbation) diagram with the following conventions:

1) Particles are represented by horizontal lines, those on the right being labelled by  $\mathbf{p}_i$ , those on the left by  $\mathbf{p}'_i$ .

2) A vertical dashed line between a pair of particle lines corresponds to a two-body interaction.

3) The  $T$  matrix is represented by a shaded blob.

The perturbation series (19.28) may then be represented diagrammatically (for  $i = 3$ ) as

$$\begin{aligned} \text{Diagram: } \mathbf{p}'_1 \text{---} \text{blob} \text{---} \mathbf{p}_1, \mathbf{p}'_2 \text{---} \text{blob} \text{---} \mathbf{p}_2 &= \text{Diagram: } \mathbf{p}'_1 \text{---} \mathbf{p}_1, \mathbf{p}'_2 \text{---} \mathbf{p}_2 + \text{Diagram: } \mathbf{p}'_1 \text{---} \text{blob} \text{---} \mathbf{p}_1, \mathbf{p}'_2 \text{---} \mathbf{p}_2 + \text{Diagram: } \mathbf{p}'_1 \text{---} \mathbf{p}_1, \mathbf{p}'_2 \text{---} \text{blob} \text{---} \mathbf{p}_2 + \dots \\ T_3 &= V^3 + V^3 G_0 V^3 + V^3 G_0 V^3 G_0 V^3 + \dots \end{aligned} \quad (19.29)$$



while the Lippmann–Schwinger equation (19.9b) reads

$$\begin{array}{c} \mathbf{p}'_1 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} \\ \mathbf{p}'_2 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} \\ T_3 = V^3 + V^3 G_0 T_3. \quad (19.30)$$

Let us now look at the three-body  $\mathcal{T}$ -operator given by eqs. (19.12)–(19.13). For example, eq. (19.13a) may be pictured as

$$\begin{array}{c} \mathbf{p}'_1 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} \\ \mathbf{p}'_2 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} \\ \mathbf{p}'_3 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_3 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_3 \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_3 \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_3 \end{array} \\ \mathcal{T} = V + V G_0 \mathcal{T} \quad (19.31)$$

where we have taken into account the fact that  $V = V^1 + V^2 + V^3$ . From eq. (19.26) we also note that the two-body Lippmann–Schwinger equation (19.9b) written in three-body space, may be represented as

$$\begin{array}{c} \mathbf{p}'_1 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_1 \end{array} \\ \mathbf{p}'_2 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_2 \end{array} \\ \mathbf{p}'_3 \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_3 \end{array} = \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} + \begin{array}{c} \text{---} \\ \hline \text{---} \end{array} \begin{array}{c} \text{---} \\ \hline \mathbf{p}_3 \end{array} \quad (19.32)$$

Diagrams such as those appearing in eq. (19.32), where one particle remains unaffected, are called *disconnected*. We shall see shortly that disconnected diagrams play an important role in the analysis of three-body problems.

## 19.2. Difficulties with the Lippmann–Schwinger equations

Let us consider the Lippmann–Schwinger equations for the Green's operator

$$G = G_0 + G_0 V G \quad (19.33a)$$

$$= G_0 + G V G_0 \quad (19.33b)$$

and for the  $\mathcal{T}$ -operator

$$\mathcal{T} = V + V G_0 \mathcal{T} \quad (19.34a)$$

$$= V + \mathcal{T} G_0 V. \quad (19.34b)$$

For *two-body* scattering the corresponding equation for the wave function, namely

$$\psi_{\mathbf{k}_1} = \Phi_{\mathbf{k}_1} + G_0 V \psi_{\mathbf{k}_1} \quad (19.35)$$

was analyzed in Chapter 5. In particular, we showed in Section 5.6 that although the original Lippmann–Schwinger kernel  $K = G_0 V$  is not square integrable ( $\mathcal{L}^2$ ), a simple manipulation (iterating once or multiplying by  $V^{1/2}$ ) leads to an equation whose kernel is  $\mathcal{L}^2$  and to which the Fredholm theory of integral equations can be applied. The result is that for two-body

scattering the Lippmann–Schwinger equation (19.35) is a “good” (well behaved) integral equation with a unique solution  $\psi_{k_1}^{(+)}$  such that in configuration space

$$\psi_{k_1}^{(+)}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ \exp(i\mathbf{k}_1 \cdot \mathbf{r}) + f(\theta, \phi) \frac{e^{ikr}}{r} \right].$$

For three-body problems we have already encountered a serious drawback of the Lippmann–Schwinger equations in Chapter 16 [see the discussion following eqs. (16.10)]. We showed indeed that the Lippmann–Schwinger equations (16.3) for the state vectors do not have a unique solution. In addition, we shall now prove that for three or more particles the kernel  $K = G_0 V$  of the Lippmann–Schwinger equation is not an  $\mathcal{L}^2$  operator [1]. To see this, let us evaluate the norm of the operator  $K$ , namely

$$\|K\| = [\text{Tr}(KK^\dagger)]^{1/2} \quad (19.36)$$

with

$$\text{Tr}(KK^\dagger) = \int |\langle \alpha' | K | \alpha \rangle|^2 d\alpha d\alpha' \quad (19.37)$$

and  $\alpha$  is a complete set of variables. We shall work here in the momentum representation, so that the matrix element appearing in eq. (19.37) is given by

$$\begin{aligned} \langle \mathbf{p}'_1 \mathbf{p}'_2 \mathbf{p}'_3 | K | \mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_3 \rangle &= \frac{\delta(\mathbf{p}'_1 + \mathbf{p}'_2 + \mathbf{p}'_3 - \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{p}_3)}{E - \sum_{i=1}^3 (p_i^2/2m_i) + i\epsilon} \\ &\times [\delta(\mathbf{p}'_1 - \mathbf{p}_1) \langle \mathbf{q}'_1 | V^1 | \mathbf{q}_1 \rangle + \delta(\mathbf{p}'_2 - \mathbf{p}_2) \langle \mathbf{q}'_2 | V^2 | \mathbf{q}_2 \rangle \\ &+ \delta(\mathbf{p}'_3 - \mathbf{p}_3) \langle \mathbf{q}'_3 | V^3 | \mathbf{q}_3 \rangle]. \end{aligned} \quad (19.38)$$

We may eliminate the total momentum conserving delta function  $\delta(\mathbf{p}'_1 + \mathbf{p}'_2 + \mathbf{p}'_3 - \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{p}_3)$  by working in the C.M. system of the three-particle system. However, the integrand of eq. (19.37) will still contain terms of the type  $[\delta(\mathbf{p}'_1 - \mathbf{p}_1)]^2$  with the result that  $\text{Tr}(KK^\dagger)$  is infinite and the kernel  $K$  is not  $\mathcal{L}^2$ . We note that this difficulty arises from the presence of *disconnected diagrams* such as those appearing in eq. (19.32). This fact, together with the non-uniqueness of the solution of the Lippmann–Schwinger equations, are entirely new features with respect to the two-body situation. They are characteristic of three (and more) particle problems.

We have shown above that the kernel  $K = G_0 V$  of the Lippmann–Schwinger equation for three-body problems is not square integrable (i.e. is not a Hilbert–Schmidt kernel). However, the mathematical theory of integral equations also yields very useful results when the kernel is *compact*. Such a kernel may be defined as follows [4]: we construct normalized (wave packet) states  $\Psi_n(\alpha)$  from a complete set of wave functions belonging to the Hilbert space of the system. The kernel  $K$  is then said to be compact (or *completely continuous*) if for any infinite set of the  $\Psi_n$  the set

$$K \Psi_n(\alpha) = \int \langle \alpha | K | \alpha' \rangle \Psi_n(\alpha') d\alpha' \quad (19.39)$$

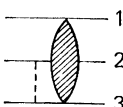
contains a subset which converges towards a limit. One should therefore investigate the possibility of the Lippmann–Schwinger kernel  $K = G_0 V$  being a compact kernel for three-body situations. This question has been studied by Faddeev [1] and Weinberg [5] who showed that the answer is negative.

### 19.3. The Faddeev equations

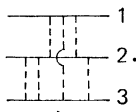
In order to remove the difficulties which we have just analyzed, Faddeev has suggested the following method. The basic idea is to write the scattering operator  $\mathcal{T}(E)$  as

$$\mathcal{T}(E) = \mathcal{T}^{(1)}(E) + \mathcal{T}^{(2)}(E) + \mathcal{T}^{(3)}(E) \quad (19.40)$$

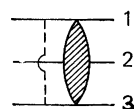
where  $\mathcal{T}^{(1)}(E)$  represents the sum of all the diagrams contributing to  $\mathcal{T}(E)$  in which particles 2 and 3 are the last to interact. In other words,  $\mathcal{T}^{(1)}$  is a scattering operator such that any three-body process has occurred (including no interaction at all), and then particles 2 and 3 interact. In terms of diagrams, we may write (we simply label the particles lines by 1, 2, 3):

$$\mathcal{T}^{(1)}(E) = \text{diagram} \quad (19.41a)$$


where the blob denotes any process occurring between the three particles. For example, a particular diagram contributing to  $\mathcal{T}^{(1)}(E)$  is



In the same way, we define

$$\mathcal{T}^{(2)}(E) = \text{diagram} \quad (19.41b)$$


and

$$\mathcal{T}^{(3)}(E) = \text{diagram} \quad (19.41c)$$


Since the sum of  $\mathcal{T}^{(1)}$ ,  $\mathcal{T}^{(2)}$  and  $\mathcal{T}^{(3)}$  obviously exhausts all the perturbation diagrams available for a three-body system, we see that eq. (19.40) immediately follows from the definitions (19.41).

Let us now analyze more carefully the content of  $\mathcal{T}^{(1)}$ . We may consider it as made of two parts. In the first one particle 1 *never* interacts with 2 or 3. The sum of these diagrams is just the two-body scattering operator  $T_1(E)$ , i.e.

$$T_1(E) = \begin{array}{c} \text{---} 1 \\ | \\ \text{---} 2 \\ | \\ \text{---} 3 \end{array} \text{ (diagram with shaded blob on line 2)} = \begin{array}{c} \text{---} 1 \\ | \\ \text{---} 2 \\ | \\ \text{---} 3 \end{array} + \begin{array}{c} \text{---} 1 \\ | \\ \text{---} 2 \\ | \\ \text{---} 3 \end{array} + \cdots \quad (19.42)$$

In the second part, an arbitrary sequence of interactions between the three particles is followed by an interaction between particles 1 and 3 (or 1 and 2), and then particles 2 and 3 interact a certain number of times. The sum of such contributions may be represented as

$$\mathcal{T}^{(1)}(E) = \begin{array}{c} \text{---} 1 \\ | \\ \text{---} 2 \\ | \\ \text{---} 3 \end{array} \text{ (diagram with shaded blob on line 2)} + \begin{array}{c} \text{---} 1 \\ | \\ \text{---} 2 \\ | \\ \text{---} 3 \end{array} \text{ (diagram with shaded blob on line 2)} \quad (19.43)$$

or [see eqs. (19.41b) and (19.41c)]

$$\mathcal{T}^{(1)}(E) = T_1 G_0 \mathcal{T}^{(2)} + T_1 G_0 \mathcal{T}^{(3)}. \quad (19.44)$$

Thus, adding up the contributions (19.42) and (19.43), we find that

$$\mathcal{T}^{(1)} = T_1 + \mathcal{T}^{(1)}$$

or, using eq. (19.44)

$$\mathcal{T}^{(1)} = T_1 + T_1 G_0 \mathcal{T}^{(2)} + T_1 G_0 \mathcal{T}^{(3)}. \quad (19.45a)$$

Similarly, we also have

$$\mathcal{T}^{(2)} = T_2 + T_2 G_0 \mathcal{T}^{(1)} + T_2 G_0 \mathcal{T}^{(3)} \quad (19.45b)$$

and

$$\mathcal{T}^{(3)} = T_3 + T_3 G_0 \mathcal{T}^{(1)} + T_3 G_0 \mathcal{T}^{(2)}. \quad (19.45c)$$

The equations (19.45) are called the *Faddeev* equations for the  $\mathcal{T}$ -operator. We may write them in matrix form as

$$\begin{pmatrix} \mathcal{T}^{(1)} \\ \mathcal{T}^{(2)} \\ \mathcal{T}^{(3)} \end{pmatrix} = \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} + \begin{pmatrix} 0 & T_1 & T_1 \\ T_2 & 0 & T_2 \\ T_3 & T_3 & 0 \end{pmatrix} G_0 \begin{pmatrix} \mathcal{T}^{(1)} \\ \mathcal{T}^{(2)} \\ \mathcal{T}^{(3)} \end{pmatrix}. \quad (19.46)$$

Before we analyze in more detail the structure of the Faddeev equations, it is important to realize that these equations may be obtained *independently of perturbation theory*. Thus, starting from the Lippmann–Schwinger equation (19.13a) for  $\mathcal{T}$ , namely

$$\mathcal{T} = V + V G_0 \mathcal{T} \quad (19.47)$$

(where  $V = V^1 + V^2 + V^3$ ) we define the operators

$$\mathcal{T}^{(1)} = V^1 + V^1 G_0 \mathcal{T} \quad (19.48a)$$

$$\mathcal{T}^{(2)} = V^2 + V^2 G_0 \mathcal{T} \quad (19.48b)$$

and

$$\mathcal{T}^{(3)} = V^3 + V^3 G_0 \mathcal{T} \quad (19.48c)$$

so that

$$\mathcal{T} = \mathcal{T}^{(1)} + \mathcal{T}^{(2)} + \mathcal{T}^{(3)}. \quad (19.49)$$

Next, we note that since the two-body operator  $T_1$  is such that

$$T_1 = V^1 + T_1 G_0 V^1$$

we may write

$$V^1 = T_1 - T_1 G_0 V^1. \quad (19.50)$$

Substituting in eq. (19.48a), we find that

$$\mathcal{T}^{(1)} = T_1 - T_1 G_0 V^1 + T_1 G_0 \mathcal{T} - T_1 G_0 V^1 G_0 \mathcal{T}$$

or

$$\begin{aligned} \mathcal{T}^{(1)} &= T_1 + T_1 G_0 \mathcal{T} - T_1 G_0 (V^1 + V^1 G_0 \mathcal{T}) \\ &= T_1 + T_1 G_0 (\mathcal{T} - \mathcal{T}^{(1)}) \end{aligned}$$

so that

$$\mathcal{T}^{(1)} = T_1 + T_1 G_0 (\mathcal{T}^{(2)} + \mathcal{T}^{(3)})$$

which is precisely eq. (19.45a). A similar reasoning leads to eqs. (19.45b) and (19.45c). We have thus obtained the Faddeev equations by pure algebraic manipulations involving the Lippmann-Schwinger equations for the two and three-body  $T$ -operators [6].

Let us now return to the Faddeev equations in matrix form, eq. (19.46). We may interpret these equations as integral equations whose kernel is a matrix operator  $[K] \equiv K_{ij}$  ( $i, j = 1, 2, 3$ ) [7]. The condition for this kernel to be square integrable now becomes

$$\text{Tr} \sum_{i,j=1}^3 (K_{ij} K_{ij}^\dagger) < \infty. \quad (19.51)$$

A casual glance at eq. (19.46) would lead one to believe that little has been gained by introducing the Faddeev kernel  $K_{ij}$ , since the two-body  $T$ -matrices which appear in it are clearly disconnected. However, we note that only the off-diagonal elements of  $K_{ij}$  contain disconnected parts, so that any iteration of the kernel will suppress the troublesome delta functions. Thus, iterating once the Faddeev equations, we obtain the new matrix equations

$$\begin{pmatrix} \mathcal{T}^{(1)} \\ \mathcal{T}^{(2)} \\ \mathcal{T}^{(3)} \end{pmatrix} = \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} + [K] \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} + [K^2] \begin{pmatrix} \mathcal{T}^{(1)} \\ \mathcal{T}^{(2)} \\ \mathcal{T}^{(3)} \end{pmatrix} \quad (19.52)$$

with

$$[K^2] = \begin{bmatrix} T_1 G_0 T_2 + T_1 G_0 T_3 & T_1 G_0 T_3 & T_1 G_0 T_2 \\ T_2 G_0 T_3 & T_2 G_0 T_1 + T_2 G_0 T_3 & T_2 G_0 T_1 \\ T_3 G_0 T_2 & T_3 G_0 T_1 & T_3 G_0 T_1 + T_3 G_0 T_2 \end{bmatrix} G_0 \quad (19.53)$$



The fact that the Faddeev equations require only two-body  $T$ -matrices (and no potentials) has been used as an incentive for generalizing these equations to relativistic three-body problems. The aim is to obtain Lorentz-invariant linear integral equations which reduce to the Faddeev equations in the non-relativistic limit, use only two-body  $T$ -matrices as input and have a unique solution satisfying three-body unitarity. Such equations have been obtained [13–15] and applied [16] to various relativistic three-body problems. Unfortunately, they do not take into account the important concept of crossing symmetry [17].

So far, we have discussed the Faddeev equations in terms of the  $T$ -operators. Similar equations may evidently be written down for the total Green's operator  $G(E)$  or for the various wave functions. Thus we have

$$G = G_0 + GVG_0 \quad (19.56)$$

or, using eq. (19.13c)

$$G = G_0 + G_0 \mathcal{T} G_0. \quad (19.57)$$

From eq. (19.40), we then obtain

$$G = G_0 + G^{(1)} + G^{(2)} + G^{(3)} \quad (19.58)$$

with

$$G^{(i)} = G_0 \mathcal{T}^{(i)} G_0. \quad (19.59)$$

The Green's operators  $G^{(i)}$  then satisfy the Faddeev equations

$$\begin{pmatrix} G^{(1)} \\ G^{(2)} \\ G^{(3)} \end{pmatrix} = \begin{pmatrix} G_1 - G_0 \\ G_2 - G_0 \\ G_3 - G_0 \end{pmatrix} + G_0 \begin{pmatrix} 0 & T_1 & T_1 \\ T_2 & 0 & T_2 \\ T_3 & T_3 & 0 \end{pmatrix} \begin{pmatrix} G^{(1)} \\ G^{(2)} \\ G^{(3)} \end{pmatrix} \quad (19.60)$$

where the Green's operators  $G_i$  are defined by eq. (19.6).

Let us now consider an eigenstate  $\Psi_a \equiv \Psi_{i,\alpha}$  of the total Hamiltonian  $H$  corresponding to the initial free state  $\Phi_a \equiv \Phi_{i,\alpha}$ . The subscript  $i$  is an arrangement channel index which may take on the values  $i = 0, 1, 2, 3$ , while the label  $\alpha$  contains the additional information on bound states, momenta, spin, isospin, . . . to complete the description of a given initial channel. By definition the value  $i = 0$  refers to three free particles in the initial state  $\Phi_{0,\alpha}$ , with

$$H = H_0 + V$$

and

$$H_0 \Phi_{0,\alpha} = E_{0,\alpha} \Phi_{0,\alpha}.$$

The case  $i = 1$  describes a situation in which initially the particle 1 is free and the pair (2, 3) is bound. This corresponds to the splitting

$$H = H_1 + V_1$$

with

$$\begin{aligned} H_1 &= H_0 + V^1 = H_0 + V_{23}, \\ V_1 &= V - V^1 = V_{12} + V_{13} \end{aligned}$$

and

$$H_1 \Phi_{1,\alpha} = E_{1,\alpha} \Phi_{1,\alpha}.$$

Similar definitions hold for the cases  $i = 2$  and  $i = 3$ .

We may now easily derive the Faddeev equations satisfied by the eigenstates  $\Psi_{i,\alpha}$ . For example, in the case  $i = 1$  one finds [1] that

$$\Psi_{1,\alpha} = \Psi^{(1)} + \Psi^{(2)} + \Psi^{(3)} \quad (19.61)$$

with

$$\begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \\ \Psi^{(3)} \end{pmatrix} = \begin{pmatrix} \Phi_{1,\alpha} \\ 0 \\ 0 \end{pmatrix} + G_0(E) \begin{pmatrix} 0 & T_1(E) & T_1(E) \\ T_2(E) & 0 & T_2(E) \\ T_3(E) & T_3(E) & 0 \end{pmatrix} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \\ \Psi^{(3)} \end{pmatrix} \quad (19.62)$$

and  $E = E_{1\alpha} + i\varepsilon$ . The solution of the inhomogeneous equation (19.62) is unique, since the corresponding homogeneous equation has solutions if and only if there is a three-body bound state at the energy  $E_{1\alpha}$ . Indeed, let us write the homogeneous equation which corresponds to the first of eqs. (19.62),

$$\Psi^{(1)} = G_0(E) T_1(E) [\Psi^{(2)} + \Psi^{(3)}]. \quad (19.63)$$

Using eq. (19.11), we have

$$\Psi^{(1)} = G_1(E) V^1 [\Psi^{(2)} + \Psi^{(3)}]. \quad (19.64)$$

Multiplying eq. (19.64) to the left by  $E - H_0 - V^1 \equiv G_1^{-1}$ , we obtain

$$(E - H_0) \Psi^{(1)} = V^1 (\Psi^{(2)} + \Psi^{(3)}) + V^1 \Psi^{(1)}$$

or

$$(E - H_0) \Psi^{(1)} = V^1 \Psi. \quad (19.65a)$$

Similarly, we find that

$$(E - H_0) \Psi^{(2)} = V^2 \Psi \quad (19.65b)$$

and

$$(E - H_0) \Psi^{(3)} = V^3 \Psi. \quad (19.65c)$$

Adding the three equations (19.65) we conclude that

$$(E - H_0 - V) \Psi = (E - H) \Psi = 0$$

if  $\Psi = \Psi^{(1)} + \Psi^{(2)} + \Psi^{(3)}$  is a solution of the homogeneous equation

$$\begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \\ \Psi^{(3)} \end{pmatrix} = G_0(E) \begin{pmatrix} 0 & T_1(E) & T_1(E) \\ T_2(E) & 0 & T_2(E) \\ T_3(E) & T_3(E) & 0 \end{pmatrix} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \\ \Psi^{(3)} \end{pmatrix}. \quad (19.66)$$

Such a solution clearly corresponds to a three-body bound state.



Let us now describe briefly some of the techniques which have been useful in attempting to solve the Faddeev equations.

First of all, we note that after separating the motion of the center of mass, the Faddeev equations are coupled linear integral equations in *six* variables. Such equations cannot be handled by present-day computers and must therefore be simplified.

An important step towards the simplification of the Faddeev equations is to separate out the total angular momentum  $J$ . This has been accomplished by Omnès [18] and reduces the Faddeev equations to a set of coupled integral equations in *three* variables.

A further simplification consists in approximating the two-body potentials – or directly the two-body transition matrix elements – by *separable* (factorable) forms (see Section 5.7). To understand how this approximation comes about, we first note that if  $E$  is near the energy of a two-body bound state  $E_{Bi}$ , the corresponding two-body  $T$ -matrix  $T_i(E)$  is dominated by a term of the separable form. Indeed, writing

$$T_i(E) = V^i + V^i G_i(E) V^i$$

and inserting a complete set of eigenstates of the Hamiltonian  $H_i = H_0 + V_i$ , we find that

$$T_i(E) = V^i + \frac{V^i |\psi_{Bi}\rangle \langle \psi_{Bi}| V^i}{E - E_{Bi}} + \int d\mathbf{q}'' \frac{V^i |\psi_{q''}\rangle \langle \psi_{q''}| V^i}{E - E_{q''} + i\epsilon} \quad (19.67)$$

where we have assumed for the sake of simplicity that there is only one bound state. Hence, when  $E$  is in the vicinity of  $E_{Bi}$ , we may write

$$\langle \mathbf{q}'_i | T_i(E) | \mathbf{q}_i \rangle \simeq \frac{g_{Bi}(\mathbf{q}'_i) g_{Bi}(\mathbf{q}_i)}{E - E_{Bi}} \quad (19.68)$$

where the “form factor”  $g_{Bi}$  is given by

$$g_{Bi}(\mathbf{q}_i) = \langle \mathbf{q}_i | V^i | \psi_{Bi} \rangle = (E_{Bi} - q_i^2/2\mu_i) \psi_{Bi}(\mathbf{q}_i) \quad (19.69)$$

and

$$\psi_{Bi}(\mathbf{q}_i) \equiv \langle \mathbf{q}_i | \psi_{Bi} \rangle \quad (19.70)$$

is the two-body bound state wave function written in momentum space.

Let us now assume that the two-body potential  $V^i$  itself contains only one factorable ( $S$ -wave) term [the generalization to several terms is straightforward], so that we may write

$$V^i = \lambda_i |v_i\rangle \langle v_i|. \quad (19.71)$$

Thus in configuration space

$$\langle \mathbf{r}' | V^i | \mathbf{r} \rangle = \lambda_i v_i(\mathbf{r}') v_i(\mathbf{r}) \quad (19.72)$$

with

$$v_i(\mathbf{r}) = \langle \mathbf{r} | v_i \rangle$$

while in momentum space

$$\langle \mathbf{q}'_i | V^i | \mathbf{q}_i \rangle = \lambda_i g_i(\mathbf{q}'_i) g_i(\mathbf{q}_i) \quad (19.73)$$

with

$$g_i(\mathbf{q}_i) = \langle \mathbf{q}_i | v_i \rangle.$$

On the other hand, the Lippmann-Schwinger equation for the (off-shell) two-body  $T$  matrix is then given by [see eq. (16.21c)]

$$\langle \mathbf{q}' | T_i(E) | \mathbf{q}_i \rangle = \lambda_i g_i(\mathbf{q}') g_i(\mathbf{q}_i) + \lambda_i g_i(\mathbf{q}') \int d\mathbf{q}'' \frac{g_i(\mathbf{q}'') \langle \mathbf{q}'' | T_i(E) | \mathbf{q}_i \rangle}{E - E_{q''} + i\varepsilon}. \quad (19.74)$$

We may solve this equation by a method entirely analogous to that given after eq. (5.149). The result is

$$\langle \mathbf{q}' | T_i(E) | \mathbf{q}_i \rangle = \lambda_i g_i(\mathbf{q}') g_i(\mathbf{q}_i) \beta_i(E) \quad (19.75)$$

where

$$\beta_i(E) = \frac{1}{1 - \lambda_i \int d\mathbf{q}'' g_i^2(\mathbf{q}'') / (E - E_{q''} + i\varepsilon)}. \quad (19.76)$$

Hence, for a factorable potential, the corresponding  $T$  matrix  $T(E)$  is also factorable. This result also holds for the partial wave  $T$  matrix which then assumes the form

$$T_{l,i}(q'_i, q_i, E) = \lambda_{l,i} g_{l,i}(q'_i) g_{l,i}(q_i) \beta_{l,i}(E) \quad (19.77)$$

with

$$\langle \mathbf{q}' | V^i | \mathbf{q}_i \rangle = \sum_{l,m} V_{l,i}(q'_i, q_i) Y_{lm}^*(\hat{\mathbf{q}}'_i) Y_{lm}(\hat{\mathbf{q}}_i),$$

$$V_{l,i}(q'_i, q_i) = \lambda_{l,i} g_{l,i}(q'_i) g_{l,i}(q_i)$$

and

$$\beta_{l,i}(E) = \frac{1}{1 - \lambda_{l,i} \int_0^\infty dq'' q''^2 g_{l,i}^2(q'') / (E - E_{q''} + i\varepsilon)}. \quad (19.78)$$

We now observe that a sharp resonance of energy  $E_r$  and width  $\Gamma$  in the partial wave  $l$  is characterized by a pole of  $T_{l,i}(q'_i, q_i, E)$  at an energy  $E = E_r - \frac{1}{2}i\Gamma$  in the second Riemann sheet. In the vicinity of this pole, the partial wave  $T$  matrix may be shown to have the form [8]

$$T_{l,i}(q'_i, q_i, E) = \frac{\tilde{g}_{l,i}(q'_i) \tilde{g}_{l,i}(q_i)}{E - E_r + \frac{1}{2}i\Gamma} \quad (19.79)$$

where  $\tilde{g}_{l,i}(q_i)$  is the resonance “form factor”. Thus we see that when the energy  $E$  is close to the energy of a bound state or of a sharp resonance the two-body  $T$ -matrix elements assume a form which can be reproduced by separable interaction potentials. These facts suggest that one may try to use separable two-body interaction potentials – leading to separable two-body  $T$  matrices, even off the energy shell – in the Faddeev equations. These equations then reduce to linear integral equations which, after partial wave analysis, are just integral equations in one variable [19].

To conclude this section we shall now derive a slightly different version of the Faddeev equations, called the *Lovelace equations* [8]. These equations involve the operators  $U_{fi}$  and  $\bar{U}_{fi}$  defined by eqs. (14.164) which lead directly to the transition matrix elements for a process  $i\alpha \rightarrow f\beta$ . We first recall that

$$U_{fi} = V_i + V_f G V_i \quad (19.80a)$$

and

$$\bar{U}_{fi} = V_f + V_f G V_i \quad (19.80b)$$

where

$$V_i = V - V^i, \quad i = 0, 1, 2, 3$$

is the interaction between the projectile and the target in the initial channel  $i$ , while

$$V_f = V - V^f, \quad f = 0, 1, 2, 3$$

is the interaction between the outgoing particles in the final channel  $f$ . For example, if  $f = 2$ , then  $V_f$  is the interaction between particle 2 and the bound pair (1, 3). The off-shell transition matrix elements for a process  $i\alpha \rightarrow f\beta$  are given by eqs. (14.165), namely

$$\begin{aligned} \langle f\beta | \mathcal{T}^{(+)} | i\alpha \rangle &= \langle \Phi_{f\beta}(E_{f\beta}) | V_f + V_f G(E_{i\alpha} + i\epsilon) V_i | \Phi_{i\alpha}(E_{i\alpha}) \rangle \\ &= \langle \Phi_{f\beta}(E_{f\beta}) | \bar{U}_{fi}(E_{i\alpha}) | \Phi_{i\alpha}(E_{i\alpha}) \rangle \end{aligned} \quad (19.81a)$$

and

$$\begin{aligned} \langle f\beta | \mathcal{T}^{(-)} | i\alpha \rangle &= \langle \Phi_{f\beta}(E_{f\beta}) | V_i + V_f G(E_{f\beta} + i\epsilon) V_i | \Phi_{i\alpha}(E_{i\alpha}) \rangle \\ &= \langle \Phi_{f\beta}(E_{f\beta}) | U_{fi}(E_{f\beta}) | \Phi_{i\alpha}(E_{i\alpha}) \rangle. \end{aligned} \quad (19.81b)$$

The physical (on-shell)  $T$  matrix is evidently obtained by setting  $E = E_{i\alpha} = E_{f\beta}$  and taking the limit  $\epsilon \rightarrow 0^+$ . It is a simple matter to establish the relationship between the Faddeev operators  $\mathcal{T}^{(i)}$  and the Lovelace operators  $U_{fi}$  and  $\bar{U}_{fi}$ . Using the Faddeev equations (19.46), one then obtains for  $\bar{U}_{fi}$  the Lovelace equations

$$\bar{U}_{fi} = V_f + \sum_{k \neq i} \bar{U}_{fk} G_0 T_k \quad (19.82a)$$

while  $U_{fi}$  satisfy the Lovelace equations

$$U_{fi} = V_i + \sum_{k \neq f} T_k G_0 U_{ki} \quad (19.82b)$$

where  $i, f, k = 1, 2, 3$  [20]. For example, if  $i = 1$ , we find that eq. (19.82b) becomes

$$\begin{aligned} U_{11} &= V_1 + T_2 G_0 U_{21} + T_3 G_0 U_{31} \\ U_{21} &= V_1 + T_1 G_0 U_{11} + T_3 G_0 U_{31} \\ U_{31} &= V_1 + T_1 G_0 U_{11} + T_2 G_0 U_{21} \end{aligned} \quad (19.83)$$

which we may also write in matrix form as

$$\begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = V_1 + \begin{pmatrix} 0 & T_2 & T_3 \\ T_1 & 0 & T_3 \\ T_1 & T_2 & 0 \end{pmatrix} G_0 \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix}. \quad (19.84)$$

We note that the (matrix) kernel of eq. (19.82a) is just the transposed Faddeev kernel appearing in eq. (19.46), so that all the results concerning the compactness properties of the (iterated) Faddeev kernel apply equally well to the Lovelace kernel.

We shall not discuss here in detail the various applications of the Faddeev–Lovelace equations to specific (non-relativistic) three-body problems. The three-nucleon problem has been analyzed by Mitra et al. [21] and by Sitenko et al. [22], who studied the triton binding energy and the doublet and quartet neutron–deuteron scattering lengths. Neutron–deuteron elastic scattering has also been studied by several authors [23].

More recently, possible applications of the Faddeev equations to a number of three-body atomic problems with Coulomb interactions have been investigated. A review of this work may be found in reference [24].

Finally, we remark that the Faddeev–Lovelace equations may be solved by iteration in order to generate *multiple scattering expansions*. We shall return to this point in the following section.

## 19.4. Multiple scattering expansions

### 19.4.1. Faddeev–Watson multiple scattering series

Let us consider a three-body scattering process in which particle 1 is initially incident on the bound pair (2, 3). The (on-shell) transition matrix element corresponding to the transition  $1\alpha \rightarrow f\beta$  is then given by

$$\langle f\beta | \mathcal{T} | 1\alpha \rangle = \langle \Phi_{f\beta} | U_{f1} | \Phi_{1\alpha} \rangle = \langle \Phi_{f\beta} | \bar{U}_{f1} | \Phi_{1\alpha} \rangle \quad (19.85)$$

where  $U_{f1}$  and  $\bar{U}_{f1}$  are the Lovelace operators defined in the preceding section. For elastic and inelastic (excitation) scattering, one has  $f = 1$  so that

$$1 + (2, 3) \rightarrow 1 + (2, 3)$$

or

$$1 + (2, 3) \rightarrow 1 + (2, 3)^*, \quad (19.86)$$

where the asterisk denotes an excited state.

For *rearrangement collisions* such as “pick-up” or “knock-out” reactions we have either  $f = 2$  or  $f = 3$  corresponding to the processes

$$1 + (2, 3) \rightarrow (1, 3) + 2, \quad f = 2 \quad (19.87)$$

and

$$1 + (2, 3) \rightarrow (1, 2) + 3, \quad f = 3. \quad (19.88)$$

Evidently the term “pick-up” or “knock-out” depends on the labelling of the particles. For example, in the reaction (19.87) the particle 3 is picked up by particle 1, while the particle 2 may be said to be “knocked-out” from the

bound system (2, 3). Usually these terms apply to the lightest particle of a bound pair [25]. Finally, the case  $f = 0$  corresponds to the *break-up process*

$$1 + (2, 3) \rightarrow 1 + 2 + 3 \quad (19.89)$$

which is also called *ionization* in the case of atomic processes.

In what follows we shall be interested in obtaining *multiple scattering expansions* [26–32] for the various transition matrix elements corresponding to direct (elastic and inelastic) scattering, rearrangement collisions and break up processes. As we shall see, such expansions are particularly useful at *high energies*, i.e. when the relative kinetic energy of the incident particle 1 with respect to the target (2, 3) is large compared to the binding energy of that target. We shall assume from now on that this high-energy condition is satisfied.

Let us start with the case  $f = 1$  and return to the Lovelace equations (19.82)–(19.84). A first iteration of eq. (19.83) yields

$$\begin{aligned} U_{21} &= V_1, & U_{31} &= V_1 \\ U_{11} &= V_1 + T_2 G_0 V_1 + T_3 G_0 V_1. \end{aligned} \quad (19.90)$$

Iterating a second time, we have

$$\begin{aligned} U_{21} &= V_1 + T_1 G_0 V_1 + T_1 G_0 T_2 G_0 V_1 + T_1 G_0 T_3 G_0 V_1 + T_3 G_0 V_1, \\ U_{31} &= V_1 + T_1 G_0 V_1 + T_1 G_0 T_2 G_0 V_1 + T_1 G_0 T_3 G_0 V_1 + T_2 G_0 V_1, \\ U_{11} &= V_1 + T_2 G_0 V_1 + T_3 G_0 V_1 + T_2 G_0 T_1 G_0 V_1 + T_2 G_0 T_3 G_0 V_1 \\ &\quad + T_3 G_0 T_1 G_0 V_1 + T_3 G_0 T_2 G_0 V_1 + \dots \end{aligned}$$

Using the fact that

$$V_1 = V - V^1 = V^2 + V^3$$

and eliminating the potentials in favour of the  $T$ -matrices by repeated use of eq. (19.9a), we find from eq. (19.85) that for elastic and inelastic scattering (where  $f = 1$ ) the relevant  $T$ -matrix element  $\langle 1\beta | \mathcal{T}_s | 1\alpha \rangle$  is given by the multiple scattering expansion

$$\langle 1\beta | \mathcal{T}_s | 1\alpha \rangle = \langle \Phi_{1\beta} | U_{11} | \Phi_{1\alpha} \rangle \quad (19.91a)$$

with

$$\begin{aligned} U_{11} &= T_2 + T_3 + T_3 G_0 T_2 + T_2 G_0 T_3 + T_2 G_0 T_1 G_0 T_2 + T_2 G_0 T_3 G_0 T_2 \\ &\quad + T_3 G_0 T_1 G_0 T_2 + T_2 G_0 T_1 G_0 T_3 + T_3 G_0 T_1 G_0 T_3 + T_3 G_0 T_2 G_0 T_3 + \dots \end{aligned} \quad (19.91b)$$

Similarly, for a rearrangement collision corresponding to the choice  $f = 3$ , namely

$$1 + (2, 3) \rightarrow (1, 2) + 3$$

we find that the  $T$  matrix is given by

$$\langle 3\beta | \mathcal{T}_R | 1\alpha \rangle = \langle \Phi_{3\beta} | U_{31} | \Phi_{1\alpha} \rangle \quad (19.92a)$$

with

$$U_{31} = V^3 + T_2 + T_1 G_0 T_2 + T_1 G_0 T_3 + T_2 G_0 T_3 + \dots \quad (19.92b)$$

For three-body break-up collisions, we must first include the channels  $i = f = 0$  in the Lovelace equations as described above (i.e. by defining  $T_0 = 0$ ). It is then a simple matter to generate a multiple scattering series for the operator  $U_{01}$ , with the result

$$\langle 0\beta | \mathcal{T}_B | 1\alpha \rangle = \langle \Phi_{0\beta} | U_{01} | \Phi_{1\alpha} \rangle \quad (19.93a)$$

and

$$U_{01} = T_2 + T_3 + T_1 G_0 T_2 + T_3 G_0 T_2 + T_1 G_0 T_3 + T_2 G_0 T_3 + \dots \quad (19.93b)$$

The rules for obtaining higher-order multiple scattering terms in the expansions (19.91)–(19.93) are easily derived:

(i) Start from the right with a two-body  $T$  matrix for any one of the pairs which participate in the initial interaction  $V_i = V - V^i$ .

(ii) Write  $G_0$  and  $T_i$  alternatively, avoiding the repetition of adjacent indices.

(iii) Terminate to the desired order with a two-body  $T$ -matrix for any of the pairs which participate in the final interaction  $V_f = V - V^f$ .

Our multiple scattering expansions (19.91)–(19.93) have been obtained thus far by using the Lovelace operators  $U_{fi}$ . Similar expansions may evidently be written down by making use of the operators  $\bar{U}_{fi}$ . For direct collisions ( $f = 1$ ) one immediately finds again eqs. (19.91), while the new rearrangement and break-up series are given respectively by

$$\bar{U}_{31} = V^1 + T_2 + T_1 G_0 T_2 + T_1 G_0 T_3 + T_2 G_0 T_3 + \dots \quad (19.92')$$

and

$$\bar{U}_{01} = V^1 + T_2 + T_3 + T_1 G_0 T_2 + T_3 G_0 T_2 + T_1 G_0 T_3 + T_2 G_0 T_3 + \dots \quad (19.93')$$

We conclude immediately by comparing eq. (19.93') with eq. (19.93b) that the term  $V^1 = V_{23}$  should not contribute to the transition matrix element, so that  $\langle \Phi_{0\beta} | V^1 | \Phi_{1\alpha} \rangle = 0$ . This may easily be verified, since

$$\langle \Phi_{0\beta} | V^1 | \Phi_{1\alpha} \rangle = \langle \Phi_{0\beta} | H_1 - H_0 | \Phi_{1\alpha} \rangle = 0.$$

Let us now comment briefly on the physical interpretation of the multiple scattering series which we have generated. First of all, we note that these multiple scattering expansions are rearrangements of the corresponding Born series. For example, in the case of elastic or inelastic scattering, corresponding to the process  $1 + (2, 3) \rightarrow 1 + (2, 3)$ , the Born series for the  $T$  matrix is given by

$$\langle 1\beta | \mathcal{T}_s | 1\alpha \rangle = \langle \Phi_{1\beta} | V_1 + V_1 G_1 V_1 + V_1 G_1 V_1 G_1 V_1 + \dots | \Phi_{1\alpha} \rangle \quad (19.94)$$

with

$$V_1 = V - V^1 = V_{12} + V_{13} = V^2 + V^3 \quad (19.95a)$$

and

$$G_1 = G_0 + G_0 V^1 G_1. \quad (19.95b)$$

Using eqs. (19.95) together with eqs. (19.8)–(19.11), we may sum the subseries in  $V^2$  and  $V^3$  appearing in eq. (19.94) to all orders in the interaction potentials. The result, expressed in terms of  $T$  matrices, is given by eqs. (19.91). Similar results hold for the rearrangement and the break-up case, leading respectively to eqs. (19.92) and (19.93).

Closely connected to the preceding remark is the fact that if we write approximately (for weak couplings)

$$T_i \simeq V^i \quad (19.96)$$

and limit our expansions (19.91)–(19.93) to the first order in the *interaction potentials*, we find that eqs. (19.91) give

$$\langle 1\beta | \mathcal{T}_s | 1\alpha \rangle \simeq \langle \Phi_{1\beta} | V^2 + V^3 | \Phi_{1\alpha} \rangle \quad (19.97a)$$

while eqs. (19.92) become

$$\langle 3\beta | \mathcal{T}_r | 1\alpha \rangle \simeq \langle \Phi_{3\beta} | V^2 + V^3 | \Phi_{1\alpha} \rangle \quad (19.97b)$$

and eqs. (19.93) yield

$$\langle 0\beta | \mathcal{T}_b | 1\alpha \rangle \simeq \langle \Phi_{0\beta} | V^2 + V^3 | \Phi_{1\alpha} \rangle. \quad (19.97c)$$

The three expressions (19.97) are just the first Born approximations for these processes (in the prior form). It is very important to note that the approximation (19.96) is obviously valid only for *weak couplings*. For any problem in which the potentials can bind particles the validity of the first Born expressions (19.97) must be examined carefully.

Let us now return to the multiple scattering expansion (19.91b) for the transition matrix corresponding to direct (elastic and inelastic) scattering. Another simple approximation consists in keeping only the terms which involve only *one* two-body  $T$ -matrix, so that

$$\mathcal{T}_s \simeq T_2 + T_3. \quad (19.98)$$

This approximation is known as the *impulse approximation* [33–38] for the process  $1 + (2, 3) \rightarrow 1 + (2, 3)$ . We note that the two-body  $T$ -matrices  $T_2$  and  $T_3$  describe the scattering of the incident particle 1 by the two target particles 2 and 3 as if those particles were *free*. The effect of the interaction  $V_{23}$  between the two target particles appears only in higher order terms of the series (19.91b). We shall return in more detail to the impulse approximation while analyzing high-energy hadron–deuteron scattering in Section 19.6.

As a final remark, we note that the multiple scattering expansions derived above may also be obtained from the Watson multiple scattering theory [38]. We shall therefore refer to these expansions as *Faddeev–Watson* multiple scattering series; they may readily be generalized to collisions involving more than three particles.

#### 19.4.2. Eikonal multiple scattering expansions

We shall now obtain multiple scattering expansions within the framework of the *eikonal approximation*. The generalization of this approximation to

many-body scattering problems is due to Glauber [39–41], who applied it extensively to high-energy hadron–nucleus collisions.

Although in Sections 19.5 and 19.6 we shall apply the Glauber theory to three-body problems, we shall formulate the method here for the more general case of a fast particle A incident on a target B which contains  $N$  scatterers.

Before we do this, however, let us first recall a few important formulae for high-energy two-body scattering in the eikonal approximation. Let  $\mathbf{r}$  be the relative coordinate of the two particles, whereas  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are the initial and final relative momenta. We choose the  $z$ -axis to be perpendicular to the wave vector transfer  $\Delta = \mathbf{k}_i - \mathbf{k}_f$  (see Section 9.1) and decompose the vector  $\mathbf{r}$  as

$$\mathbf{r} = \mathbf{b} + z\hat{\mathbf{z}} \quad (19.99)$$

where  $\mathbf{b}$  is the “impact parameter” vector, perpendicular to the  $z$ -direction. The scattering amplitude is then given in the eikonal approximation by [see eq. (9.37)]

$$f_E = \frac{k}{2\pi i} \int d^2\mathbf{b} \exp(i\Delta \cdot \mathbf{b}) (\exp\{i\chi(\mathbf{b})\} - 1) \quad (19.100)$$

where  $k = |\mathbf{k}_i| = |\mathbf{k}_f|$  and  $\chi(\mathbf{b})$  is the phase shift function. [In order to simplify the notation we do not write explicitly the  $k$ -dependence of  $\chi$ .] Defining the quantity

$$\Gamma(\mathbf{b}) = 1 - \exp[i\chi(\mathbf{b})] \quad (19.101)$$

we may rewrite eq. (19.100) as

$$f_E = \frac{ik}{2\pi} \int d^2\mathbf{b} \exp(i\Delta \cdot \mathbf{b}) \Gamma(\mathbf{b}). \quad (19.102)$$

It is important to remark that the derivation of eq. (19.100) does not require the existence of a potential to describe the collision process. As we already showed in Chapter 9, it is sufficient to sum the partial wave series in the high-energy, small angle limit to obtain eq. (19.100).

The basic expression (19.100) has been obtained in the C.M. system of the two colliding particles. However, for high-energy small angle scattering eq. (19.100) may easily be shown to retain its validity in the laboratory system [42]. The only modification is that  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are now replaced by the initial and final momenta  $\mathbf{k}_L$  and  $\mathbf{k}'_L$  of the projectile in the laboratory frame. Of course, the magnitude of  $\mathbf{k}'_L$  is now smaller than that of  $\mathbf{k}_L$  because of recoil effects, but the energy transfer (which is proportional to the square of the momentum transfer) is very small for scattering near the forward direction. We shall neglect it in what follows and evaluate the laboratory two-body scattering amplitudes for  $k_L = k'_L$ .

We now consider the scattering of a fast particle A by a composite target B containing  $N$  scatterers. We assume that the motion of the target particles is



slow by comparison with the relative motion of A and B. Moreover, we suppose that the incident particle interacts with the target scatterers by means of two-body spin-independent interactions. We also neglect possible exchange effects between the incident and target particles. The Glauber scattering amplitude for a direct collision leading from an initial target state  $|0\rangle$  to a final state  $|m\rangle$  is then given in the center of mass system by

$$f_{m0}^G = \frac{k_i}{2\pi i} \int d^2b \exp(i\mathbf{A} \cdot \mathbf{b}) \langle m | [\exp\{i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)\} - 1] | 0 \rangle \quad (19.103)$$

the corresponding differential cross section being such that

$$\frac{d\sigma_{m0}^G}{d\Omega} = \frac{k_f}{k_i} |f_{m0}^G|^2. \quad (19.104)$$

Here  $\mathbf{A} = \mathbf{k}_i - \mathbf{k}_f$  is the C.M. wave vector transfer, while

$$\mathbf{r} = \mathbf{b} + z\hat{\mathbf{z}} \quad (19.105)$$

is the initial relative coordinate and

$$\mathbf{r}_j = \mathbf{b}_j + z_j\hat{\mathbf{z}} \quad (19.106)$$

are the coordinates of the target particles (with respect to the target center of mass). The  $z$ -axis may be chosen along  $\mathbf{k}_i$  for small angle collisions, but we shall also consider other choices below, in particular the one which consists in taking  $\hat{\mathbf{z}}$  to be perpendicular to  $\mathbf{A}$ . The total Glauber phase shift function

$$\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N) = \sum_{j=1}^N \chi_j(\mathbf{b} - \mathbf{b}_j) \quad (19.107)$$

is the sum of the phase shifts  $\chi_j$  contributed by each of the target scatterers as the wave representing the incident particle progresses through the target system. This crucial property of *phase-shift additivity* is clearly a direct consequence of the one-dimensional nature of the relative motion, together with the neglect of three-body forces, target scatterer motion and longitudinal momentum transfer.

It is important to note that the Glauber expression (19.103) only applies to collisions for which the energy transfer  $\Delta E$  is small compared with the incident particle energy  $E_i$ . This is true for elastic collisions and for “mildly” inelastic ones in which the target is excited or perhaps breaks up. It is not true for “deeply” inelastic collisions in which the nature of the incident or target particles is modified or the number of particles is altered during the collision. We shall leave aside such processes in what follows. We also note that if we neglect recoil effects (which are small near the forward direction) we may write the Glauber scattering amplitude in the laboratory system as

$$f_{m0}^G = \frac{k_L}{2\pi i} \int d^2b \exp(i\mathbf{q} \cdot \mathbf{b}) \langle m | [\exp\{i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)\} - 1] | 0 \rangle \quad (19.108)$$

where  $\mathbf{q} = \mathbf{k}_L - \mathbf{k}'_L$  is now the laboratory wave vector transfer. This last expression is more suitable for the analysis of high-energy hadron-nucleus

collisions because we want the nuclei to remain non-relativistic and we also wish to use directly hadron-nucleon data in order to study hadron-nucleus collisions.

Following Glauber [40], we define the quantity

$$\Gamma_{\text{tot}}(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N) = 1 - \exp[i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)] \quad (19.109)$$

so that eq. (19.108) becomes

$$f_{m0}^G = \frac{ik_L}{2\pi} \int d^2\mathbf{b} \exp(i\mathbf{q} \cdot \mathbf{b}) \langle m | \Gamma_{\text{tot}}(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N) | 0 \rangle. \quad (19.110)$$

Let us now introduce the objects

$$\Gamma_j(\mathbf{b} - \mathbf{b}_j) = 1 - \exp[i\chi_j(\mathbf{b} - \mathbf{b}_j)]. \quad (19.111)$$

Because of eqs. (19.107) and (19.109), we may write

$$\Gamma_{\text{tot}} = 1 - \prod_{j=1}^N [1 - \Gamma_j(\mathbf{b} - \mathbf{b}_j)] \quad (19.112)$$

or

$$\Gamma_{\text{tot}} = \sum_{j=1}^N \Gamma_j - \sum_{j \neq l} \Gamma_j \Gamma_l + \dots + (-1)^{N-1} \prod_{j=1}^N \Gamma_j. \quad (19.113)$$

This last equation, when substituted into eq. (19.110), leads directly to an interesting interpretation of the collision in terms of a multiple scattering expansion. Indeed, by inverting eq. (19.102), one may obtain the quantities  $\Gamma_j$  in terms of the two-body scattering amplitudes describing the scattering of the incident particle by the  $j$ th scatterer [43]. Hence, the terms linear in  $\Gamma_j$  on the right-hand side of eq. (19.113) account for the “single scattering” (impulse) approximation to the scattering amplitude, whereas the next terms provide double, triple, . . . scattering corrections. We note that the order of multiple scattering can at most be  $N$ , reflecting the fact that the scattering is focused in the forward direction.

It is important to realize that the Glauber generalization of the eikonal method described above makes no reference to interaction *potentials*. Only the two-body phase shift functions  $\chi_j$  (or the functions  $\Gamma_j$ ) must be known in order to obtain  $\Gamma_{\text{tot}}$ . This fact makes the Glauber theory particularly useful for analyzing hadronic collisions, in particular high-energy hadron-nucleus scattering, as we shall illustrate in Sections 19.6 and 20.3.

If the basic two-body interactions are known, as in atomic physics, we can actually obtain the eikonal scattering amplitude in terms of these interaction potentials. For example, let us consider the non-relativistic scattering of a charged, “elementary” particle by an atom. Working in the center of mass system, we write the full, many-body eikonal wave function as a generalization of the expression (9.30), namely

$$\Psi_E(\mathbf{r}, X) = (2\pi)^{-3/2} \exp\left[i\mathbf{k}_i \cdot \mathbf{r} - \frac{i}{\hbar v_i} \int_{-\infty}^z V_i(\mathbf{b}, z', X) dz'\right] \psi(X). \quad (19.114)$$

Here  $\mathbf{r}$  is the initial relative coordinate,  $\mathbf{v}_i = \hbar \mathbf{k}_i / M_i$  is the initial relative velocity (with  $M_i$  being the reduced mass in the initial channel) and the symbol  $X$  denotes collectively the target coordinates. The potential  $V_i$  is the full initial channel interaction between the incident particle and all the scatterers in the target. The corresponding eikonal transition matrix element is then given by eq. (14.157) in which the exact scattering state vector  $\Psi_a^{(+)}$  is replaced by  $\Psi_E$ . Thus

$$\langle b | \mathcal{T} | a \rangle \simeq \langle \Phi_b | V_i | \Psi_E \rangle. \quad (19.115)$$

Clearly, a similar formula may be obtained by using the exact expression  $\langle \Psi_b^{(-)} | V_i | \Phi_a \rangle$  [see eq. (14.157)] and replacing in it the state vector  $\Psi_b^{(-)}$  by the corresponding eikonal wave function (whose phase now contains  $V_f$ , the full interaction between the outgoing particles in the final state). Calling  $\Psi'_E$  this eikonal wave function, we then have also

$$\langle b | \mathcal{T} | a \rangle \simeq \langle \Psi'_E | V_i | \Phi_a \rangle. \quad (19.116)$$

Let us now return to eq. (19.115). For a *direct* collision (such that  $V_i = V_f = V_d$ ) leading from an initial target state  $|0\rangle$  to a final target state  $|m\rangle$ , we deduce from eq. (15.54) that the *many-body eikonal scattering amplitude* is given by

$$f_{m0} = -\frac{M}{2\pi\hbar^2} \int d^2\mathbf{b} \, d\mathbf{z} \exp(i\mathbf{A} \cdot \mathbf{r}) \left\langle m \left| V_d(\mathbf{b}, \mathbf{z}, X) \exp \left[ -\frac{i}{\hbar v_i} \int_{-\infty}^z V_d(\mathbf{b}, \mathbf{z}', X) dz' \right] \right| 0 \right\rangle, \quad (19.117)$$

where  $M = M_i = M_f$ .

For *elastic* scattering processes such that  $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ , and if we choose the  $z$ -axis to be perpendicular to  $\mathbf{A}$ , we may perform the  $z$ -integral in eq. (19.117) to obtain the Glauber result [cf. eq. (19.103) with  $|m\rangle \equiv |0\rangle$ ]

$$f_{el}^G = \frac{k}{2\pi i} \int d^2\mathbf{b} \exp(i\mathbf{A} \cdot \mathbf{b}) \langle 0 | [\exp\{i\chi_{tot}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)\} - 1] | 0 \rangle \quad (19.118)$$

with

$$\chi_{tot}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N) = -\frac{1}{\hbar v_i} \int_{-\infty}^{+\infty} V_d(\mathbf{b}, \mathbf{z}, X) dz. \quad (19.119)$$

We remark that for *inelastic* (direct) processes the Glauber scattering amplitude (19.103) can only be obtained from the more general expression (19.117) by neglecting the longitudinal momentum transfer. Indeed,  $\mathbf{A}$  now lies *along*  $\mathbf{k}_i$  (and not perpendicular to it) in the case of forward scattering.

Instead of generating a multiple scattering series in terms of the quantities  $\Gamma_j$  (which in turn may be obtained in terms of two-body scattering amplitudes) we may also obtain from eq. (19.103) another multiple scattering series which is more closely related to the one we have analyzed in Section 9.1

within the framework of non-relativistic potential scattering. As an example, let us consider the case of elastic scattering for which we write the Glauber amplitude (19.118) as

$$f_{\text{el}}^{\text{G}} = \sum_{n=1}^{\infty} \bar{f}_{\text{G}n} \quad (19.120)$$

where

$$\bar{f}_{\text{G}n} = \frac{k}{2\pi i} \frac{i^n}{n!} \int d^2\mathbf{b} \exp(i\mathbf{A} \cdot \mathbf{b}) \langle 0 | [\chi_{\text{tot}}^{\text{G}}(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)]^n | 0 \rangle. \quad (19.121)$$

As in the case of potential scattering, it is interesting to compare the Glauber series (19.120) with the corresponding Born series

$$f_{\text{el}} = \sum_{n=1}^{\infty} \bar{f}_{\text{B}n}. \quad (19.122)$$

Here  $\bar{f}_{\text{B}n}$ , the term of order  $n$  of the Born series, contains  $n$  times the full interaction  $V_d$  between the incident particle and the target. We immediately note that if the Glauber phase shift function  $\chi_{\text{tot}}^{\text{G}}$  is evaluated along a  $z$ -axis perpendicular to  $\mathbf{A}$ , then

$$\bar{f}_{\text{G}1} = \bar{f}_{\text{B}1}. \quad (19.123)$$

Higher terms of the Born and Glauber series will be examined below (see Sections 19.5 and 21.1) for the case of elastic electron-atom scattering.

## 19.5. Electron-hydrogen collisions

As a first example of a realistic three-body problem, we shall now give a brief account of electron collisions with atomic hydrogen. Such processes have been extensively studied by numerous theoretical methods [44]. We shall only discuss here a few of them which have proved to be particularly useful.

### 19.5.1. Preliminaries

Let us first establish some basic formulae pertaining to electron-hydrogen scattering. We shall denote respectively by  $\mathbf{r}_0$  and  $\mathbf{r}_1$  the coordinates of the "incident" and the "atomic" electron with respect to the (infinitely heavy) proton. In what follows we shall also neglect spin-dependent interactions (which are very small). Thus the spins of the two electrons will only influence the scattering through the Pauli principle and the spin of the proton will be neglected. We assume that in the initial state the hydrogen atom is in the ground state, described (in atomic units [45]) by the wave function

$$\psi_0(\mathbf{r}_1) = \frac{1}{\sqrt{\pi}} \exp(-r_1).$$

The free electron in the initial state, having a wave vector  $\mathbf{k}_i$  and a spin orientation  $v_0$  is described by the wave function

$$\phi_{\mathbf{k}_i, v_0} = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \chi_{v_0}(s_0) \quad (19.124)$$

where  $s_0$  is the spin variable of the incident electron. We shall also use the notation

$$\begin{aligned} \chi_{1/2}(s_0) &\equiv \alpha(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \chi_{-1/2}(s_0) &\equiv \beta(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned} \quad (19.125)$$

If we denote by  $\chi_{v_1}(s_1)$  the spin eigenvector of the atomic electron, corresponding to the spin orientation  $v_1$ , we see that the complete unsymmetrized free wave describing the initial state is given by

$$\Phi_a = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_0(r_1) \chi_{v_0}(s_0) \chi_{v_1}(s_1) \quad (19.126)$$

while the corresponding energy is given by

$$E_a = \hbar^2 k_i^2 / 2m + w_0, \quad w_0 = -e^2 / 2a_0$$

or, in atomic units

$$E_a = \frac{1}{2} k_i^2 + w_0, \quad w_0 = -\frac{1}{2}. \quad (19.127)$$

For example, if both electrons have initially "spin up", we have

$$\Phi_a = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_0(r_1) \alpha(0) \alpha(1).$$

We note that the free wave  $\Phi_a$  is an eigenvector of the initial arrangement channel Hamiltonian

$$H_i = -\frac{1}{2} \nabla_{\mathbf{r}_0}^2 - \frac{1}{2} \nabla_{\mathbf{r}_1}^2 - \frac{1}{r_1}. \quad (19.128)$$

The complete Hamiltonian of the system is given by

$$H = -\frac{1}{2} \nabla_{\mathbf{r}_0}^2 - \frac{1}{2} \nabla_{\mathbf{r}_1}^2 - \frac{1}{r_0} - \frac{1}{r_1} + \frac{1}{r_{01}} \quad (19.129)$$

with  $r_{01} = |\mathbf{r}_0 - \mathbf{r}_1|$ . Thus the interaction potential in the initial channel is

$$V_i = H - H_i = -\frac{1}{r_0} + \frac{1}{r_{01}}. \quad (19.130)$$

Let us now consider some possible (unsymmetrized) *final* free states of the system. For elastic scattering we have

$$\Phi_b = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_0(r_1) \chi_{v'_0}(s_0) \chi_{v'_1}(s_1) \quad (19.131)$$

and conservation of energy requires that

$$E_b = \frac{1}{2} k_f^2 + w_0; \quad k_f = k_i, \quad w_0 = -\frac{1}{2}.$$

For direct excitation to the state  $|n\rangle$ , one has

$$\Phi_b = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(r_1) \chi_{v'_0}(s_0) \chi_{v'_1}(s_1) \quad (19.132)$$

and conservation of energy yields

$$E_b = \frac{1}{2}k_f^2 + w_n = \frac{1}{2}k_i^2 + w_0.$$

We note that both free states (19.131) or (19.132) are eigenstates of the arrangement channel Hamiltonian (19.128). For direct scattering we thus have

$$H_f \Phi_b = E_b \Phi_b \quad (19.133a)$$

with

$$H_f = H_i = H_d \quad (19.133b)$$

and

$$V_f = V_i = V_d = -\frac{1}{r_0} + \frac{1}{r_{01}}. \quad (19.133c)$$

We now examine *exchange* scattering, for which the incident electron takes the place of the atomic one. We then have in the final channel

$$H_f = -\frac{1}{2}\nabla_{r_0}^2 - \frac{1}{2}\nabla_{r_1}^2 - \frac{1}{r_0}, \quad (19.134a)$$

$$V_f = H - H_f = -\frac{1}{r_1} + \frac{1}{r_{01}} \equiv V_p. \quad (19.134b)$$

If the hydrogen atom is left in the ground state, the final free state is given by

$$\Phi_{pb} = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_0(r_0) \chi_{v_0}(s_1) \chi_{v_1}(s_0) \quad (19.135)$$

with

$$H_f \Phi_{pb} = E_b \Phi_{pb}.$$

Conservation of energy then gives

$$E_b = \frac{1}{2}k_f^2 + w_0, \quad k_f = k_i, \quad w_0 = -\frac{1}{2}.$$

For the excitation to the state  $|n\rangle$ , we have

$$\Phi_{pb} = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(r_0) \chi_{v_0}(s_1) \chi_{v_1}(s_0) \quad (19.136)$$

with the energy-conserving relation

$$E_b = \frac{1}{2}k_f^2 + w_n = \frac{1}{2}k_i^2 + w_0.$$

According to the general equation (16.160), the correctly symmetrized transition matrix element which we need in this case is

$$\bar{T}_{ba} = T_{ba}^d - T_{ba}^{ex}. \quad (19.137)$$

Here the *direct* transition matrix element (on-the-energy-shell  $E = E_a = E_b$ ) is given by

$$T_{ba}^d = \left\langle \Phi_b \left| V_d + V_d \frac{1}{E - H + i\varepsilon} V_d \right| \Phi_a \right\rangle \quad (19.138a)$$

$$= \langle \Phi_b | V_d | \Psi_a^{(+)} \rangle \quad (19.138b)$$

$$= \langle \Psi_b^{(-)} | V_d | \Phi_a \rangle \quad (19.138c)$$

with

$$\Psi_a^{(+)} = \Phi_a + \frac{1}{E - H + i\varepsilon} V_d \Phi_a. \quad (19.138d)$$

On the other hand, the *exchange* transition matrix element (on-the-energy-shell) is such that

$$T_{ba}^{ex} = \left\langle \Phi_{Pb} \left| V_P \text{ (or } V_d) + V_P \frac{1}{E - H + i\varepsilon} V_d \right| \Phi_a \right\rangle \quad (19.139a)$$

$$= \langle \Phi_{Pb} | V_P | \Psi_a^{(+)} \rangle \quad (19.139b)$$

$$= \langle \Psi_{Pb}^{(-)} | V_d | \Phi_a \rangle \quad (19.139c)$$

where

$$\Psi_{Pb}^{(-)} = \Phi_{Pb} + \frac{1}{E - H - i\varepsilon} V_P \Phi_{Pb} \quad (19.139d)$$

and [see eq. (14.159)]

$$\langle \Phi_{Pb} | V_P | \Phi_a \rangle = \langle \Phi_{Pb} | V_d | \Phi_a \rangle. \quad (19.139e)$$

Let us analyze eq. (19.137) in more detail. We assume for the moment that the incident electron has spin “up”. If the incident and atomic electrons have parallel spins before and after the collision while the hydrogen atom is left in the state  $|n\rangle$  (with  $|n\rangle \equiv |0\rangle$  for elastic scattering), we have

$$\bar{T}_{ba}(\uparrow\uparrow \rightarrow \uparrow\uparrow) = T_{ba}^d(\uparrow\uparrow \rightarrow \uparrow\uparrow) - T_{ba}^{ex}(\uparrow\uparrow \rightarrow \uparrow\uparrow) \quad (19.140)$$

where, according to eqs. (19.138)

$$\begin{aligned} T_{ba}^d(\uparrow\uparrow \rightarrow \uparrow\uparrow) &= \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(\mathbf{r}_1) \alpha(0) \alpha(1) | V_d | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \alpha(0) \alpha(1) \rangle \\ &= \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(\mathbf{r}_1) | V_d | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \rangle \equiv \hat{T}_{ba}^d. \end{aligned} \quad (19.141)$$

Here we have separated the full wave function  $\Psi_a^{(+)}$  into its space and spin parts as

$$\Psi_a^{(+)} = \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \alpha(0) \alpha(1)$$

and denoted by  $\hat{T}_{ba}^d$  the direct matrix element from which the spin dependence has been removed. Similarly, we find from eqs. (19.139) that

$$T_{ba}^{ex}(\uparrow\uparrow \rightarrow \uparrow\uparrow) = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(\mathbf{r}_0) | V_P | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \rangle \equiv \hat{T}_{ba}^{ex} \quad (19.142)$$

where  $\hat{T}_{ba}^{ex}$  is the exchange matrix element from which we have eliminated the spin dependence.

Next, let us consider the case where the two electrons have antiparallel spins. We then find that

$$\begin{aligned} T_{ba}^d(\uparrow\downarrow \rightarrow \uparrow\downarrow) &= \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(\mathbf{r}_1) \alpha(0) \beta(1) | V_d | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \alpha(0) \beta(1) \rangle \\ &= \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(\mathbf{r}_1) | V_d | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \rangle = \hat{T}_{ba}^d \end{aligned}$$

while

$$T_{ba}^{ex}(\uparrow\downarrow \rightarrow \uparrow\downarrow) = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(\mathbf{r}_0) \alpha(1) \beta(0) | V_P | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \alpha(0) \beta(1) \rangle = 0.$$

Thus

$$\bar{T}_{ba}(\uparrow\downarrow \rightarrow \uparrow\downarrow) = \hat{T}_{ba}^d. \quad (19.143)$$

Finally, for spin-flip scattering, we have

$$T_{ba}^d(\uparrow\downarrow \rightarrow \downarrow\uparrow) = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(\mathbf{r}_1) \beta(0) \alpha(1) | V_d | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \alpha(0) \beta(1) \rangle = 0$$

and

$$T_{ba}^{ex}(\uparrow\downarrow \rightarrow \downarrow\uparrow) = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(\mathbf{r}_0) \beta(1) \alpha(0) | V_P | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \alpha(0) \beta(1) \rangle = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(\mathbf{r}_0) | V_P | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \rangle = \hat{T}_{ba}^{ex}$$

so that

$$\bar{T}_{ba}(\uparrow\downarrow \rightarrow \downarrow\uparrow) = \hat{T}_{ba}^{ex}. \quad (19.144)$$

To obtain the differential cross section associated with each of these (non-relativistic) processes, we insert the properly symmetrized transition matrix element  $\bar{T}_{ba}$  in eq. (15.48). Using atomic units, we then have

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} |\bar{T}_{ba}|^2. \quad (19.145a)$$

Thus, from eqs. (19.140)–(19.142) we find that

$$\frac{d\sigma}{d\Omega}(\uparrow\uparrow \rightarrow \uparrow\uparrow) = (2\pi)^4 \frac{k_f}{k_i} |\hat{T}_{ba}^d - \hat{T}_{ba}^{ex}|^2 \quad (19.145b)$$

while eq. (19.143) yields

$$\frac{d\sigma}{d\Omega}(\uparrow\downarrow \rightarrow \uparrow\downarrow) = (2\pi)^4 \frac{k_f}{k_i} |\hat{T}_{ba}^d|^2 \quad (19.145c)$$

and eq. (19.144) gives

$$\frac{d\sigma}{d\Omega}(\uparrow\downarrow \rightarrow \downarrow\uparrow) = (2\pi)^4 \frac{k_f}{k_i} |\hat{T}_{ba}^{ex}|^2. \quad (19.145d)$$

Finally, let us consider the important case where the beam and target are unpolarized and no attempt is made to distinguish between the various final spin states. The differential cross section corresponding to such a situation is given by

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \left[ \frac{d\sigma}{d\Omega}(\uparrow\uparrow \rightarrow \uparrow\uparrow) + \frac{d\sigma}{d\Omega}(\uparrow\downarrow \rightarrow \uparrow\downarrow) + \frac{d\sigma}{d\Omega}(\uparrow\downarrow \rightarrow \downarrow\uparrow) \right]$$

or

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} \frac{1}{2} [|\hat{T}_{ba}^d - \hat{T}_{ba}^{ex}|^2 + |\hat{T}_{ba}^d|^2 + |\hat{T}_{ba}^{ex}|^2]. \quad (19.146)$$



In terms of the direct and exchange *scattering amplitudes* which are given respectively by

$$f_{ba} = - (2\pi)^2 \hat{T}_{ba}^d \quad (\text{in a.u.})$$

and

$$g_{ba} = - (2\pi)^2 \hat{T}_{ba}^{ex} \quad (\text{in a.u.})$$

we may also write eq. (19.146) as

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \frac{k_f}{k_i} [|f_{ba}|^2 + |g_{ba}|^2 + |f_{ba} - g_{ba}|^2]. \quad (19.147)$$

This formula may be easily interpreted by recalling that particles with different spin components are distinguishable. Thus in half the collisions, the two electrons have different spin orientations, so that the differential cross section is simply the sum  $(k_f/k_i)|f_{ba}|^2 + (k_f/k_i)|g_{ba}|^2$  of the direct and exchange cross sections. In the other half the two electrons are truly indistinguishable, so that an antisymmetric space function must be used, leading to the scattering amplitude  $f_{ba} - g_{ba}$ . It is also worth noting that eq. (19.147) may be written as

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} [\frac{1}{4}|f_{ba} + g_{ba}|^2 + \frac{3}{4}|f_{ba} - g_{ba}|^2]. \quad (19.148)$$

Thus we verify that for a random mixture of initial spin states and all final spin states the cross section must be computed with a *symmetric* spatial wave function in *one quarter* of the cases and with an *antisymmetric* spatial wave function in the remaining *three quarters*. This is clearly a direct consequence of the *Pauli principle*, which requires that the wave function of a system of identical fermions must be completely antisymmetric. Indeed the *only* antisymmetric spin function corresponding to the singlet ( $S = 0$ ) state of the two-electron system considered here is given by

$$\frac{1}{\sqrt{2}}[\alpha(0)\beta(1) - \alpha(1)\beta(0)].$$

This spin function must multiply a symmetric spatial wave function  $\psi^{S=0}(\mathbf{r}_0, \mathbf{r}_1)$  such that  $\psi^{S=0}(\mathbf{r}_0, \mathbf{r}_1) = \psi^{S=0}(\mathbf{r}_1, \mathbf{r}_0)$ . On the other hand, the *three* symmetric spin functions corresponding to the triplet ( $S = 1$ ) state, namely

$$\begin{aligned} &\alpha(0) \alpha(1) \\ &\beta(0) \beta(1) \\ &\frac{1}{\sqrt{2}}[\alpha(0)\beta(1) + \alpha(1)\beta(0)] \end{aligned}$$

must multiply an antisymmetric spatial wave function  $\psi^{S=1}(\mathbf{r}_0, \mathbf{r}_1)$  [such that  $\psi^{S=1}(\mathbf{r}_0, \mathbf{r}_1) = -\psi^{S=1}(\mathbf{r}_1, \mathbf{r}_0)$ ].

### 19.5.2. The scattering of fast electrons by atomic hydrogen.

#### First order calculations.

We shall now compute a few typical electron-atomic hydrogen cross sections in the case that the incident electrons have a large kinetic energy with respect to the binding energy of the target. Expressed in atomic units, this condition means that

$$k_i^2 \gg 1. \quad (19.149)$$

For example, when  $k_i = 3$ , the kinetic energy of the incident electron is given by  $k_i^2/2 = 4.5$  a.u. which is about 120 eV.

We shall show below that when the condition (19.149) is satisfied, *exchange effects are relatively small* so that – as one would expect on physical grounds – direct collisions dominate at high energies. For this reason we shall first calculate various high-energy electron-hydrogen cross sections by neglecting exchange effects.

Let us now consider in more detail the direct transition matrix element  $\hat{T}_{ba}^d$  corresponding to a collision in which the hydrogen atom, initially in the state  $|0\rangle$ , is left in the state  $|n\rangle$ . It is given by eq. (19.141), namely

$$\hat{T}_{ba}^d = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_n(\mathbf{r}_1) | V_d | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \rangle \quad (19.150)$$

with

$$V_d = 1/r_{01} - 1/r_0.$$

Since we are considering the high-energy region such that the condition (19.149) applies, it is reasonable, as a plausible starting point, to evaluate the *direct T-matrix element* (19.150) in *first Born approximation* [see Chapter 8 where high-energy (non-relativistic) potential scattering is discussed]. This procedure is justified in many, but not all circumstances [46]. Thus we write

$$\psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \simeq \Phi_a(\mathbf{r}_0, \mathbf{r}_1) = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_0(r_1)$$

so that

$$\hat{T}_{ba}^d(\text{Born}) = (2\pi)^{-3} \int \exp(i\Delta \cdot \mathbf{r}_0) \psi_n^*(\mathbf{r}_1) \left[ \frac{1}{r_{01}} - \frac{1}{r_0} \right] \psi_0(r_1) d\mathbf{r}_0 d\mathbf{r}_1 \quad (19.151)$$

where the momentum transfer  $\Delta$  (expressed in atomic units) is such that

$$\Delta = \mathbf{k}_i - \mathbf{k}_f. \quad (19.152)$$

Defining the objects

$$A_{n0}(\mathbf{r}_0) = \left\langle n \left| \frac{1}{r_{01}} - \frac{1}{r_0} \right| 0 \right\rangle \quad (19.153)$$

we may also write

$$\hat{T}_{ba}^d(\text{Born}) = (2\pi)^{-3} \int \exp(i\Delta \cdot \mathbf{r}_0) A_{n0}(\mathbf{r}_0) d\mathbf{r}_0. \quad (19.154)$$

Hence, after evaluating the quantities  $A_{n0}$  we have just to perform a simple Fourier integral (as in the case of potential scattering, see Chapter 8) in order to obtain the direct Born transition matrix.

An alternative method consists in first evaluating the integral on  $\mathbf{r}_0$  appearing in eq. (19.151) by using the fact that

$$\int \frac{\exp(i\mathbf{A} \cdot \mathbf{r}_0)}{r_{01}} d\mathbf{r}_0 = \frac{4\pi}{A^2} \exp(i\mathbf{A} \cdot \mathbf{r}_1). \quad (19.155)$$

The integral on the variable  $\mathbf{r}_1$ , involving the bound state wave functions, is then performed afterwards.

Let us illustrate these formulae on a few typical processes.

i) *Elastic scattering*

In this case the quantity

$$A_{00}(r_0) = \left\langle 0 \left| \frac{1}{r_{01}} - \frac{1}{r_0} \right| 0 \right\rangle = V_{st}(r_0)$$

is just the average (static) potential felt by the incident electron in the field of the hydrogen atom. This quantity is easily evaluated in the following way. We first write, using the explicit form of  $\psi_0(\mathbf{r}_1)$ ,

$$V_{st}(r_0) = \frac{1}{\pi} \int \exp(-2r_1) \left( \frac{1}{r_{01}} - \frac{1}{r_0} \right) d\mathbf{r}_1. \quad (19.156)$$

Next, we develop the quantity  $r_{01}^{-1}$  in spherical harmonics as

$$\frac{1}{r_{01}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} \frac{(r_<)^l}{(r_>)^{l+1}} Y_{lm}(\hat{\mathbf{r}}_0) Y_{lm}^*(\hat{\mathbf{r}}_1) \quad (19.157)$$

where  $r_>$  is the greater of  $r_0$  and  $r_1$ , and  $r_<$  the lesser of them. Because the function  $\exp(-2r_1)$  appearing in eq. (19.156) does not depend on the angular variables of  $\mathbf{r}_1$ , we may easily perform the angular integrations. Only the first term on the right of eq. (19.157) – corresponding to  $l = m = 0$  – contributes to the integral and

$$V_{st}(r_0) = 4 \int_0^{\infty} dr_1 r_1^2 \exp(-2r_1) \left[ \frac{1}{r_>} - \frac{1}{r_0} \right]$$

where we have used the fact that  $Y_{00} = (4\pi)^{-1/2}$ . Breaking the integration in two parts as

$$\int_0^{\infty} = \int_0^{r_0} + \int_{r_0}^{\infty}$$

we then have

$$V_{st}(r_0) = 4 \int_{r_0}^{\infty} dr_1 r_1^2 \exp(-2r_1) \left[ \frac{1}{r_1} - \frac{1}{r_0} \right].$$

This last integral is easily performed with the result

$$V_{st}(r_0) = - (1 + 1/r_0) \exp(-2r_0). \quad (19.158)$$

We note that the static potential (19.158) which is *real* and of *short range* does not include several important features of the collision. For example, it does not take into account the *polarization* of the atom due to the presence of the incident electron. Moreover, at energies above the first excitation threshold of the target the static potential (19.158), which has no imaginary part does not account for the removal of incident particles from the initial (elastic) channel. Finally, *exchange* effects are not present in the static potential. We shall return to these questions in Section 20.4.

It is worth noting, however, that for small values of  $r_0$  the static potential (19.158) correctly reduces to the bare Coulomb interaction  $-1/r_0$  acting between the incident electron and the proton. We therefore expect that the static interaction (19.158) will govern the elastic (direct) collisions involving small distances  $r_0$ . Hence, when  $k_i \gg 1$  and if exchange effects can be neglected, the static interaction (19.158) will give an adequate description of *large angle* elastic scattering which precisely involves small impact parameters.

Let us now calculate the transition matrix element. Using eqs. (19.154) and (19.158), we have

$$\hat{T}_{ei}^d(\text{Born}) = - (2\pi)^{-3} \int \exp(i\mathbf{A} \cdot \mathbf{r}_0) \exp(-2r_0) \left(1 + \frac{1}{r_0}\right) d\mathbf{r}_0. \quad (19.159)$$

The angular integrals are easily performed by expanding the plane wave  $\exp(i\mathbf{A} \cdot \mathbf{r}_0)$  in Legendre polynomials or in spherical harmonics as

$$\exp(i\mathbf{A} \cdot \mathbf{r}_0) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(\Delta r_0) P_l\left(\frac{\mathbf{A} \cdot \mathbf{r}_0}{\Delta r_0}\right) \quad (19.160a)$$

or

$$\exp(i\mathbf{A} \cdot \mathbf{r}_0) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(\Delta r_0) Y_{lm}(\hat{\mathbf{A}}) Y_{lm}^*(\hat{\mathbf{r}}_0). \quad (19.160b)$$

Since the rest of the integrand in eq. (19.159) is spherically symmetric, only the first term of the expansions (19.160) has to be taken into account, so that

$$\hat{T}_{ei}^d(\text{Born}) = - (2\pi)^{-3} 4\pi \int_0^{\infty} dr_0 r_0^2 j_0(\Delta r_0) \exp(-2r_0) \left(1 + \frac{1}{r_0}\right) \quad (19.161)$$

with  $j_0(x) = \sin x/x$ . The integral (19.161) is now easily performed, and yields

$$\hat{T}_{ei}^d(\text{Born}) = - (2\pi^2)^{-1} \left[ \frac{\Delta^2 + 8}{(\Delta^2 + 4)^2} \right]. \quad (19.162)$$

For elastic scattering we have  $|\mathbf{k}_i| = |\mathbf{k}_f| = k$  and the length  $\Delta$  of the vector  $\mathbf{A}$  is given from eq. (19.152) by

$$\Delta = 2k \sin \frac{1}{2}\theta, \quad (19.163)$$

where  $\theta$  is the scattering angle between the vectors  $\mathbf{k}_i$  and  $\mathbf{k}_f$ .

Using eq. (19.146) we may then write the differential cross section for elastic scattering without exchange in first Born approximation as

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{el}} = (2\pi)^4 |\hat{T}_{\text{el}}^{\text{d}}(\text{Born})|^2 = 4 \frac{(\Delta^2 + 8)^2}{(\Delta^2 + 4)^4}$$

or

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{el}} = \frac{(k^2 \sin^2 \frac{1}{2}\theta + 2)^2}{4(k^2 \sin^2 \frac{1}{2}\theta + 1)^4}. \quad (19.164)$$

The corresponding (Born) total cross section  $\sigma_{\text{tot}}^{\text{el}}$  is given by

$$\sigma_{\text{tot}}^{\text{el}} = 2\pi \int_0^\pi d\theta \sin \theta \left(\frac{d\sigma}{d\Omega}\right)_{\text{el}} \quad (19.165)$$

or, since  $\Delta d\Delta = k^2 \sin \theta d\theta$

$$\sigma_{\text{tot}}^{\text{el}} = \frac{2\pi}{k^2} \int_0^{2k} d\Delta \Delta \left(\frac{d\sigma(\Delta)}{d\Omega}\right)_{\text{el}}.$$

This last integral is easily performed, with the result

$$\sigma_{\text{tot}}^{\text{el}} = \pi \frac{7k^4 + 18k^2 + 12}{3(1 + k^2)^3}. \quad (19.166)$$

We note that as  $k$  becomes large we have

$$\sigma_{\text{tot}}^{\text{el}} \simeq \frac{7\pi}{3} \frac{1}{k^2} \quad (19.167)$$

so that, as in the case of potential scattering (see Section 8.2)

$$\sigma_{\text{tot}}^{\text{el}} \underset{E \rightarrow \infty}{\sim} A E_e^{-1} \quad (19.168)$$

where  $A$  is a constant and  $E_e = \frac{1}{2}k^2$  is the kinetic energy of the incident electron (in atomic units).

The differential and total first Born elastic cross sections (19.164) and (19.166) are illustrated respectively in Figs. 19.2 and 19.3.

## ii) 1s-2s excitation

We now evaluate the quantity

$$A_{2s,1s}(\mathbf{r}_0) = \left\langle 2s \left| \frac{1}{r_{01}} - \frac{1}{r_0} \right| 1s \right\rangle \quad (19.169)$$

where

$$\psi_{2s}(r_1) = \frac{1}{4\sqrt{2}\pi} (2 - r_1) \exp(-\frac{1}{2}r_1).$$

Because of the orthogonality of the functions  $\psi_{1s}(r_1)$  and  $\psi_{2s}(r_1)$  the term  $\langle 2s | 1/r_0 | 1s \rangle$  vanishes. Thus

$$A_{2s,1s}(\mathbf{r}_0) = \frac{1}{4\pi\sqrt{2}} \int \exp(-\frac{3}{2}r_1) (2 - r_1) \frac{1}{r_{01}} d\mathbf{r}_1.$$

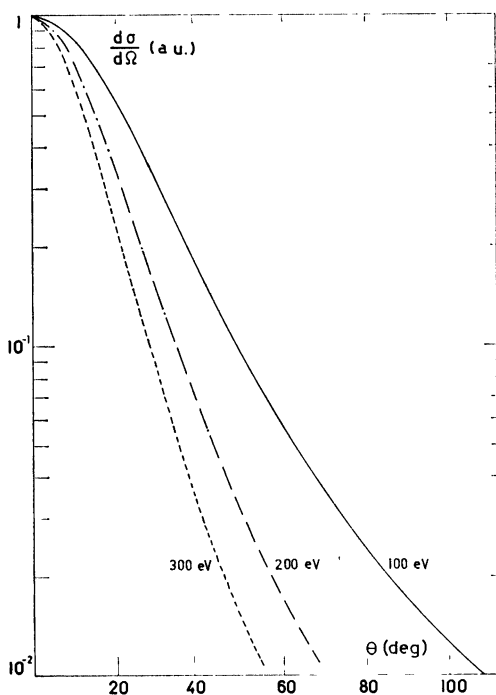


Fig. 19.2. The first Born differential cross section for elastic scattering of electrons by atomic hydrogen (without exchange) as a function of the scattering angle  $\theta$ , for 100 eV, 200 eV and 300 eV incident electrons.

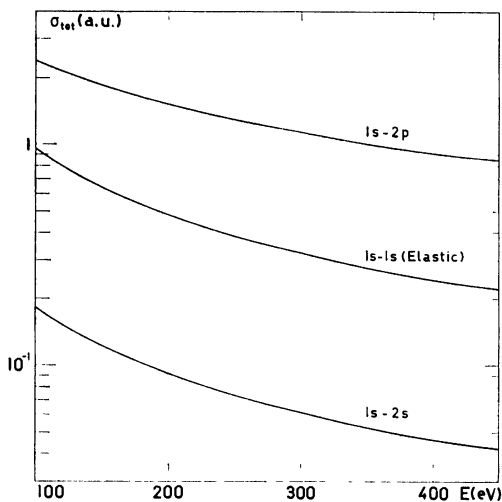


Fig. 19.3. The first Born total cross sections for elastic,  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  electron-atomic hydrogen collisions (without exchange) as a function of the incident electron energy.

This expression is easily evaluated by expanding  $r_0^{-1}$  in spherical harmonics, with the result

$$A_{2s,1s}(r_0) = \frac{4}{9\sqrt{2}} \exp(-\frac{3}{2}r_0)(r_0 + \frac{2}{3}).$$

Hence

$$\begin{aligned} \hat{T}_{2s,1s}^d(\text{Born}) &= (2\pi)^{-3} \frac{4}{9\sqrt{2}} \int \exp(i\mathbf{A} \cdot \mathbf{r}_0) \exp(-\frac{3}{2}r_0)(r_0 + \frac{2}{3}) d\mathbf{r}_0 \\ &= (2\pi)^{-3} \frac{16\pi\sqrt{2}}{(\Delta^2 + \frac{9}{4})^3} \end{aligned} \quad (19.170)$$

so that

$$\left(\frac{d\sigma}{d\Omega}\right)_{2s,1s} = \frac{k_f}{k_i} \frac{128}{(\Delta^2 + \frac{9}{4})^6}. \quad (19.171)$$

Here  $k_i$  and  $k_f$  are related by

$$\frac{1}{2}k_i^2 + w_{1s} = \frac{1}{2}k_f^2 + w_{2s}$$

or

$$\frac{1}{2}k_i^2 - \frac{1}{2} = \frac{1}{2}k_f^2 - \frac{1}{8}$$

so that

$$k_f = (k_i^2 - \frac{3}{4})^{1/2}.$$

Furthermore, if  $\theta$  is the scattering angle between the vectors  $\mathbf{k}_i$  and  $\mathbf{k}_f$ , we have

$$\Delta = (k_i^2 + k_f^2 - 2k_i k_f \cos \theta)^{1/2}.$$

The first Born differential cross section (19.171) is illustrated in Fig. 19.4 for several incident electron energies.

It is worth noting that the first Born transition matrix element (19.170) falls off like  $\Delta^{-6}$  for large momentum transfers, i.e. much faster than the first Born *elastic* transition matrix element (19.162), which behaves like  $\Delta^{-2}$  for large  $\Delta$ . However, it may be shown that the imaginary part of the *second* Born term corresponding to the transition  $1s \rightarrow 2s$  behaves like  $k^{-1}\Delta^{-2}$  for large  $k$  and large  $\Delta$ , so that the second Born term dominates the scattering at high energies and large momentum transfers. This is in accordance with the remark made in [46].

Let us now return to the first Born differential cross section (19.171). The corresponding *total* first Born cross section is given by

$$\sigma_{\text{tot}}^{2s,1s} = 2\pi \frac{128}{k_i^2} \int_{k_i - k_f}^{k_i + k_f} d\Delta \Delta \frac{1}{(\Delta^2 + \frac{9}{4})^6} \quad (19.172)$$

where we have used the fact that  $\Delta d\Delta = k_i k_f \sin \theta d\theta$ . Although this integral is readily evaluated analytically, we shall only be interested here in its leading term at high energies.

We first note that most of the contribution to this integral arises from the region near the lower limit of integration (i.e. the region of low momentum transfers) where the first Born approximation precisely governs the scattering at high (non-relativistic) energies. Moreover, since  $k_f^2 \gg 1$ , we may write

$$k_f = (k_i^2 - \frac{3}{4})^{1/2} \simeq k_i(1 - \frac{3}{8k_i^2} + \dots)$$

so that

$$k_i - k_f \simeq \frac{3}{8k_i}$$

and

$$k_i + k_f \simeq 2k_i.$$

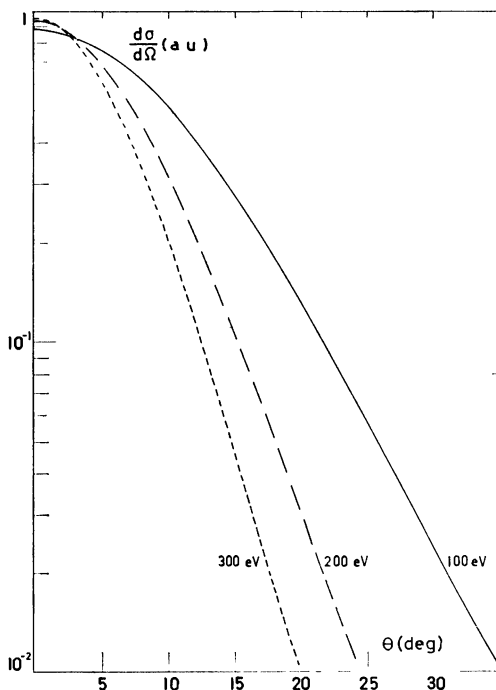


Fig. 19.4. The first Born differential cross section for excitation of the 2s state of hydrogen by electron impact (without exchange) as a function of the scattering angle  $\theta$ , for 100, 200 and 300 eV incident electrons.

Since most of the integral arises from the region of low momentum transfers and because

$$(k_i - k_f)^2 \simeq \frac{9}{64k_i^2} \ll \frac{9}{4}$$



we may obtain the leading term of the total cross section at high energies by taking the limits of integration to be 0 and  $\infty$ . Then

$$\sigma_{\text{tot}}^{2s,1s} \simeq 2\pi \frac{128}{k_i^2} \int_0^\infty d\Delta \Delta \frac{1}{(\Delta^2 + \frac{9}{4})^6}$$

or

$$\sigma_{\text{tot}}^{2s,1s} \simeq \frac{128\pi}{5} \left(\frac{2}{3}\right)^{10} \frac{1}{k_i^2}. \quad (19.173)$$

Again we observe that this cross section falls off like  $E_e^{-1}$  for large  $E_e$ . Furthermore, by comparing eqs. (19.167) and (19.173) we see that the asymptotic total cross section for 1s–2s excitation is about five times smaller than the corresponding asymptotic elastic cross section. The total first Born cross section for 1s–2s excitation is shown in Fig. 19.3.

### iii) 1s–2p excitation

Although the calculation of the 1s–2p excitation cross section may be performed as above by first evaluating  $A_{2p,1s}$  and then  $\hat{T}_{2p,1s}^d(\text{Born})$ , we shall apply here another method, in which the integration on the variable  $\mathbf{r}_0$  is performed first. We return therefore to eq. (19.151) which yields in this case

$$\hat{T}_{2p,1s}^d(\text{Born}) = (2\pi)^{-3} \int \exp(i\Delta \cdot \mathbf{r}_0) \psi_{2p}^*(\mathbf{r}_1) \frac{1}{r_{01}} \psi_{1s}(\mathbf{r}_1) d\mathbf{r}_0 d\mathbf{r}_1.$$

We note that the term  $r_0^{-1}$  in the integrand of eq. (19.151) does not contribute because of the orthogonality of  $\psi_{2p}$  and  $\psi_{1s}$ . Then, using eq. (19.155), we find that

$$\hat{T}_{2p,1s}^d(\text{Born}) = \frac{1}{2\pi^2 \Delta^2} \int \psi_{2p}^*(\mathbf{r}_1) \exp(i\Delta \cdot \mathbf{r}_1) \psi_{1s}(\mathbf{r}_1) d\mathbf{r}_1. \quad (19.174)$$

More generally, for any inelastic transition leading from the initial state  $|0\rangle$  to the final state  $|n\rangle$  of our hydrogen atom target we have [47]

$$\hat{T}_{n,0}^d(\text{Born}) = \frac{1}{2\pi^2 \Delta^2} \int \psi_n^*(\mathbf{r}_1) \exp(i\Delta \cdot \mathbf{r}_1) \psi_0(\mathbf{r}_1) d\mathbf{r}_1. \quad (19.175)$$

The integral (19.174) is readily performed by choosing the quantization axis to lie along the momentum transfer  $\Delta$ . Then the factors  $\exp(\pm i\phi_1)$  that appear in the wave functions for the magnetic substates  $m = \pm 1$  of the state  $|2p\rangle$  prevent those substates from being excited (by integration over the angle  $\phi_1$ ). The only final substate which is excited (within the framework of the first Born approximation) is then the state  $2p(m=0)$  [which is also called  $2p_0$  or  $2p_z$ ]. Its wave function is given by

$$\psi_{2p_z}(\mathbf{r}_1) = \frac{1}{2^{3/2}\sqrt{3}} r_1 \exp(-\frac{1}{2}r_1) Y_{1,0}(\hat{\mathbf{r}}_1)$$

with

$$Y_{1,0}(\hat{p}_1) = \sqrt{\frac{3}{4\pi}} \cos \theta_1.$$

Hence the transition matrix element (19.174) is given by

$$\hat{T}_{2p,1s}^d(\text{Born}) = (2\pi)^{-3} \frac{24\pi\sqrt{2}}{\Delta(\Delta^2 + \frac{9}{4})^3} i. \quad (19.176)$$

Note that this expression is purely imaginary. The corresponding first Born differential cross section is then

$$\left(\frac{d\sigma}{d\Omega}\right)_{2p,1s} = \frac{k_f}{k_i} \frac{288}{\Delta^2(\Delta^2 + \frac{9}{4})^6} \quad (19.177)$$

with

$$k_f = (k_i^2 - \frac{3}{4})^{1/2}.$$

Because of the presence of the factor  $\Delta^{-2}$ , this cross section exhibits at small angles a stronger peak than the one corresponding to the elastic or the

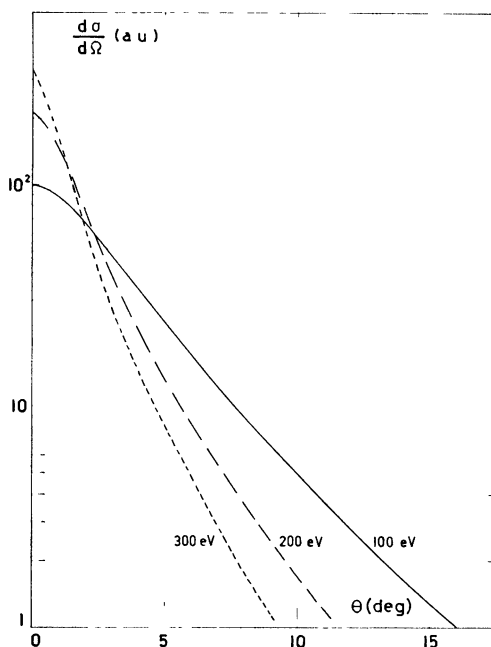


Fig. 19.5. The first Born differential cross section for excitation of the 2p state of hydrogen by electron impact (without exchange) as a function of the scattering angle  $\theta$ , for 100, 200 and 300 eV incident electrons.

1s–2s differential cross sections. For large momentum transfers we note that the first Born transition matrix element (19.176) falls off like  $\Delta^{-7}$ , i.e. much faster than the elastic first Born transition matrix element (19.162).

However, it may be proved that the *second Born* term corresponding to the transition  $1s \rightarrow 2p$  governs the scattering at high energies and large momentum transfers. This dominance of the second Born term, which we already encountered above in the case of the  $1s \rightarrow 2s$  transition, is a general feature of high-energy *inelastic* electron–atom collisions occurring at large momentum transfers.

Returning to the first Born differential cross section (19.177), we see that the *total* cross section for  $1s \rightarrow 2p$  excitation is given in the first Born approximation by

$$\sigma_{\text{tot}}^{2p,1s} = 2\pi \frac{288}{k_i^2} \int_{k_i - k_f}^{k_i + k_f} d\Delta \frac{1}{\Delta(\Delta^2 + \frac{9}{4})^6}. \quad (19.178)$$

The above integral is easily evaluated analytically. However, as for the  $1s \rightarrow 2s$  transition, we shall only be interested in obtaining the *leading term* of the cross section at high energies. As in the case of the 1s–2s excitation, we note that most of the contribution to this integral arises precisely from the region of small momentum transfers, where the first Born approximation dominates the scattering at high energies.

It is clear from eq. (19.178) that the leading term of this expression at high energies cannot be obtained by simply setting the lower limit of the integral to be zero, since the integrand is singular at  $\Delta = 0$ . Instead, let us introduce a fixed wave number  $\bar{k}$  and break the integral (19.178) in two parts as

$$\int_{k_i - k_f}^{k_i + k_f} = \int_{k_i - k_f}^{\bar{k}} + \int_{\bar{k}}^{k_i + k_f}.$$

Taking the upper limit to be  $+\infty$ , we may then write the right-hand side of eq. (19.178) as the sum of two terms, namely

$$\sigma_{\text{tot}}^{2p,1s} = \text{I} + \text{II} \quad (19.179a)$$

where

$$\text{I} = \frac{576\pi}{k_i^2} \int_{k_i - k_f}^{\bar{k}} \frac{d\Delta}{\Delta} \frac{1}{(\Delta^2 + \frac{9}{4})^6} \quad (19.179b)$$

and

$$\text{II} = \frac{576\pi}{k_i^2} \int_{\bar{k}}^{\infty} \frac{d\Delta}{\Delta} \frac{1}{(\Delta^2 + \frac{9}{4})^6}. \quad (19.179c)$$

The leading term of I is easily evaluated to give

$$\text{I} \simeq \frac{576\pi}{k_i^2} \left(\frac{2}{3}\right)^{12} [\log \bar{k} - \log(k_i - k_f)].$$

Furthermore, since  $k_i - k_f \simeq 3/(8k_i)$ , we have for large  $k_i$

$$I \simeq \frac{576\pi}{k_i^2} \left(\frac{2}{3}\right)^{12} \log k_i.$$

On the other hand, since the integral appearing in eq. (19.179c) is just a constant  $C$ , we have

$$II = \frac{576\pi}{k_i^2} C.$$

Hence, for large  $k_i$  the term  $I$  dominates the total cross section and we have

$$\sigma_{\text{tot}}^{2p,1s} \simeq 576\pi \left(\frac{2}{3}\right)^{12} \frac{\log k_i}{k_i^2}, \quad (19.180)$$

a result which in terms of the (large) incident electron energy  $E_e = \frac{1}{2}k_i^2$  may also be written as

$$\sigma_{\text{tot}}^{2p,1s} \simeq 144\pi \left(\frac{2}{3}\right)^{12} \frac{\log E_e}{E_e}. \quad (19.181)$$

The above quantity is often referred to as the Bethe-Born cross section [48-49]. We note that, unlike the elastic and 1s-2s cross sections which decrease like  $E_e^{-1}$  at high energies, the high-energy total cross section for 1s-2p excitation (which is an "optically allowed" transition) behaves like  $(\log E_e)/E_e$ , i.e. decreases less rapidly with increasing energies than the "forbidden" transitions 1s-1s or 1s-2s (see Fig. 19.3). This result is in fact more general: "optically allowed" transitions dominate the total cross section for electron-atom collisions at high energies.

Having studied in some detail several direct processes, we now consider briefly *exchange effects* in high-energy electron-hydrogen scattering. The transition matrix to be evaluated is now

$$\hat{T}_{ba}^{\text{ex}} = \langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(\mathbf{r}_0) | V_P | \psi_a^{(+)}(\mathbf{r}_0, \mathbf{r}_1) \rangle \quad (19.182)$$

where

$$V_P = 1/r_{01} - 1/r_1.$$

Since the matrix element (19.182) corresponds to a rearrangement process, it is more difficult to find a suitable approximation for it, even at high energies. We first observe that  $\hat{T}_{ba}^{\text{ex}} = 0$  if the electron-electron interaction  $r_{01}^{-1}$  is neglected. Indeed, in that case the full wave function  $\psi_a^{(+)}$  would simply be the product of a Coulomb wave  $\psi_c^{(+)}(\mathbf{r}_0)$  in the variable  $\mathbf{r}_0$  times a bound state hydrogenic wave function  $\psi_o(\mathbf{r}_1)$ . The orthogonality of the functions  $\psi_c(\mathbf{r}_0)$  and  $\psi_n(\mathbf{r}_0)$  would then yield the result  $\hat{T}_{ba}^{\text{ex}} = 0$ . Therefore, if we return to eq. (19.139a) and neglect multiple scattering terms we tentatively write, to first order in the interaction  $1/r_{01}$ ,

$$\hat{T}_{ba}^{\text{ex}} \simeq \hat{T}_{ba}^{(1)} = \left\langle (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_n(\mathbf{r}_0) \left| \frac{1}{r_{01}} \right| (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_o(\mathbf{r}_1) \right\rangle. \quad (19.183)$$

As an example of such knock-out (exchange) amplitudes, let us evaluate the following first order *elastic exchange* amplitude

$$\hat{T}_{\text{el,ex}}^{(1)} = (2\pi)^{-3} \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}_1) \psi_{1s}(r_0) \frac{1}{r_{01}} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_{1s}(r_1) d\mathbf{r}_0 d\mathbf{r}_1. \quad (19.184)$$

Writing [see eqs. (5.27) and (5.30)]

$$\frac{1}{r_{01}} = \frac{1}{2\pi^2} \int d\kappa \frac{\exp\{i\kappa \cdot (\mathbf{r}_1 - \mathbf{r}_0)\}}{\kappa^2} \quad (19.185)$$

and performing the Fourier integrals over the variables  $\mathbf{r}_0$  and  $\mathbf{r}_1$ , we have

$$\hat{T}_{\text{el,ex}}^{(1)} = \frac{4}{\pi^4} \int d\kappa \frac{1}{\kappa^2} \frac{1}{(1 + |\kappa - \mathbf{k}_i|^2)^2} \frac{1}{(1 + |\kappa - \mathbf{k}_f|^2)^2}. \quad (19.186)$$

This integral can be evaluated exactly by using the Feynman parametrization method (see Appendix D) which we used in Chapter 8 to compute the second Born approximation for the Yukawa potential. Note however that if  $k = |\mathbf{k}_i| = |\mathbf{k}_f|$  is large (as we assume here), we may obtain the *leading term* of  $\hat{T}_{\text{el,ex}}^{(1)}$  as follows. We first change the variable of integration in eq. (19.186) to  $\mathbf{q} = \kappa - \mathbf{k}_i$ . Thus

$$\hat{T}_{\text{el,ex}}^{(1)} = \frac{4}{\pi^4} \int d\mathbf{q} \frac{1}{(\mathbf{q} + \mathbf{k}_i)^2} \frac{1}{(1 + q^2)^2} \frac{1}{(1 + |\mathbf{q} + \mathbf{A}|^2)^2} \quad (19.187)$$

where  $\mathbf{A} = \mathbf{k}_i - \mathbf{k}_f$  is the momentum transfer. The leading term of this expression for large  $k$  is usually called the Ochkur approximation [50] for elastic exchange scattering. Denoting this term by  $T_{\text{el}}^{\text{Och}}$ , we have

$$T_{\text{el}}^{\text{Och}} = \frac{4}{\pi^4 k^2} \int d\mathbf{q} \frac{1}{(1 + q^2)^2} \frac{1}{(1 + |\mathbf{q} + \mathbf{A}|^2)^2}. \quad (19.188)$$

The angular integrations can now be directly performed, with the result

$$T_{\text{el}}^{\text{Och}} = \frac{4}{\pi^3 k^2 \Delta} \int_0^\infty dq \frac{q}{(1 + q^2)^2} \left[ \frac{1}{1 + (q - \Delta)^2} - \frac{1}{1 + (q + \Delta)^2} \right]$$

or

$$T_{\text{el}}^{\text{Och}} = \frac{2}{\pi^3 k^2 \Delta} \int_{-\infty}^{+\infty} dq \frac{q}{(1 + q^2)^2} \left[ \frac{1}{1 + (q - \Delta)^2} - \frac{1}{1 + (q + \Delta)^2} \right]. \quad (19.189)$$

This last integral is readily computed by contour integration and yields

$$T_{\text{el}}^{\text{Och}} = \frac{8}{\pi^2 k^2} \frac{1}{(\Delta^2 + 4)^2}. \quad (19.190)$$

We may also express the above results in terms of exchange *scattering amplitudes*. Thus the first order elastic exchange scattering amplitude is

given by  $g_{\text{el}}^{(1)} = -(2\pi)^2 \hat{T}_{\text{el,ex}}^{(1)}$  and the corresponding Ochkur approximation  $g_{\text{el}}^{\text{Och}}$  reads

$$g_{\text{el}}^{\text{Och}} = -\frac{32}{k^2} \frac{1}{(\Delta^2 + 4)^2}. \quad (19.191)$$

We remark that for fixed  $\Delta$  these Ochkur expressions fall off like  $k^{-2}$  for large  $k$ . In particular, we see that for small angle scattering the Ochkur term (19.190) is of order  $k^{-2}$  with respect to the direct elastic quantity  $\hat{T}_{\text{el}}^{\text{d}}$  given by eq. (19.162). A detailed study of higher order terms shows that the Ochkur expression (19.190) actually provides the *leading exchange* correction arising in *elastic* scattering at small angles [51]. We also note from eqs. (19.145d) and (19.190) that a pure “elastic” spin-flip differential cross section falls off like  $k^{-4}$  (or  $E_{\text{e}}^{-2}$ ) when  $\Delta$  is not too large. The corresponding pure “elastic” spin-flip *total* cross section decreases like  $k^{-6}$  (or  $E_{\text{e}}^{-3}$ ) at high energies. Since the total cross section for *direct* elastic scattering behaves like  $E_{\text{e}}^{-1}$  for large  $E_{\text{e}}$  [see eq. (19.168)] we see that exchange effects are indeed relatively small at high energies.

Let us now return to the Ochkur expression  $T_{\text{el}}^{\text{Och}}$ . Using eq. (19.188) and denoting by  $\tilde{\psi}_{1s}$  the Fourier transform of the function  $\psi_{1s}$ , we may write

$$T_{\text{el}}^{\text{Och}} = \frac{1}{2\pi^2 k^2} \int \tilde{\psi}_{1s}^*(\mathbf{q}) \tilde{\psi}_{1s}(\mathbf{q} + \Delta) d\mathbf{q}. \quad (19.192)$$

More generally, for a transition leading from the target state  $|0\rangle$  to the state  $|n\rangle$ , we have

$$T_{n,0}^{\text{Och}} = \frac{1}{2\pi^2 k_i^2} \int \tilde{\psi}_n^*(\mathbf{q}) \tilde{\psi}_0(\mathbf{q} + \Delta) d\mathbf{q} \quad (19.193)$$

and we recall that  $k_i \simeq k_f$  since we are dealing with the high-energy region. Returning to configuration space, we may also write eq. (19.193) in the form

$$T_{n,0}^{\text{Och}} = \frac{1}{2\pi^2 k_i^2} \int \exp(i\Delta \cdot \mathbf{r}) \psi_n^*(\mathbf{r}) \psi_0(\mathbf{r}) d\mathbf{r}. \quad (19.194)$$

Since the first Born inelastic ( $n \neq 0$ ) *direct* transition matrix element is given by eq. (19.175), one has

$$T_{n,0}^{\text{Och}} = \frac{\Delta^2}{k_i^2} \hat{T}_{n,0}^{\text{d}}(\text{Born}) \quad (n \neq 0) \quad (19.195a)$$

or, in terms of the corresponding scattering amplitudes,

$$g_{n,0}^{\text{Och}} = \frac{\Delta^2}{k_i^2} f_{n,0}(\text{Born}) \quad (n \neq 0) \quad (19.195b)$$

with

$$f_{n,0} = -(2\pi)^2 \hat{T}_{n,0}^{\text{d}} \quad \text{and} \quad g_{n,0}^{\text{Och}} = -(2\pi)^2 T_{n,0}^{\text{Och}}.$$

We remark that if the scattering angle  $\theta$  is of the order of  $(w_n - w_0)/E_c$  or less (i.e. of order  $k_i^{-2}$ ) then  $\Delta$  is of order  $k_i^{-1}$  and  $T_{n,0}^{\text{Och}}$  ( $n \neq 0$ ) becomes very small at small angles. For example, using eq. (19.170) we see that at small angles  $T_{2s,1s}^{\text{Och}}$  behaves like  $k_i^{-4}$ . This "accidental" smallness of the expression  $T_{n,0}^{\text{Och}}$  at small angles suggests that higher terms of the Born series (for exchange) should play here an important role [52] so that the Ochkur approximation (or any first order approximation in the interaction  $r_0^{-1}$ ) is in fact inadequate to treat inelastic exchange scattering at small momentum transfers. Moreover, it may be shown that for large  $k_i$  and large  $\Delta$  the Ochkur term  $T_{n,0}^{\text{Och}}$  is negligible with respect to the second Born term of the Born series for exchange scattering.

### 19.5.3. Multiple scattering treatment of electron collisions with hydrogen atoms

We now examine how the first order calculations described above may be improved, particularly at intermediate energies (corresponding roughly to incident electron wave numbers  $k_i$  such that  $1 < k_i \lesssim 10$ ). We begin by considering *elastic* collisions and compare the Born and Glauber series [53]. Neglecting first exchange effects (to which we shall return shortly), we recall that the Born series for the elastic direct scattering amplitude may be written as

$$f_{\text{el}}^{\text{d}} = \sum_{n=1}^{\infty} \bar{f}_{\text{B}n} \quad (19.196)$$

where (in a.u.)

$$\bar{f}_{\text{B}n} = -(2\pi)^2 \langle \mathbf{k}_f, 0 | V_d G_d^{(+)} V_d \dots G_d^{(+)} V_d | \mathbf{k}_i, 0 \rangle. \quad (19.197)$$

In this expression the potential  $V_d$  which appears  $n$  times is given by eq. (19.133c), while the Green's operator  $G_d^{(+)}$  is such that

$$G_d^{(+)} = \frac{1}{E - H_d + i\epsilon} \quad (19.198)$$

where  $H_d$  is the direct Hamiltonian [see eqs. (19.128) and (19.133b)]. We have also written the asymptotic initial and final free states (which are eigenstates of  $H_d$ ) respectively as  $|\mathbf{k}_i, 0\rangle$  and  $|\mathbf{k}_f, 0\rangle$ . A general eigenstate of  $H_d$  will be denoted by  $|\mathbf{k}, n\rangle$  and our normalization is such that [54]

$$\langle \mathbf{k}', n' | \mathbf{k}, n \rangle = \delta_{nn'} \delta(\mathbf{k} - \mathbf{k}'). \quad (19.199)$$

With these normalization conventions, and recalling that  $E = \frac{1}{2}k^2 + w_0$  (in a.u.), the second order term of the Born series may be written as

$$\bar{f}_{\text{B}2} = 8\pi^2 \int d\mathbf{k} \sum_n \frac{\langle \mathbf{k}_f, 0 | V_d | \mathbf{k}, n \rangle \langle \mathbf{k}, n | V_d | \mathbf{k}_i, 0 \rangle}{\kappa^2 - k^2 + 2(w_n - w_0) - i\epsilon} \quad (19.200)$$

where the summation over the index  $n$  evidently implies an integration when states belonging to the continuum are concerned. A useful approximation

for the expression (19.200) may be obtained by replacing the energy differences ( $w_n - w_0$ ) by an average excitation energy  $\bar{w}$ . The sum on intermediate states can then be done by closure. Thus one obtains in this way the *simplified second Born approximation* (SB2)

$$\bar{f}_{\text{SB2}} = 8\pi^2 \int d\mathbf{k} \frac{1}{\kappa^2 - k'^2 - i\epsilon} \langle 0 | \{ \langle \mathbf{k}_f | V_d | \mathbf{k} \rangle \langle \mathbf{k} | V_d | \mathbf{k}_i \rangle \} | 0 \rangle \quad (19.201)$$

with  $k'^2 = k^2 - 2\bar{w}$ . After performing the integration on the plane wave part of the matrix elements one obtains

$$\begin{aligned} \bar{f}_{\text{SB2}} = & \frac{2}{\pi^2} \int d\mathbf{k} \frac{1}{\kappa^2 - k'^2 - i\epsilon} \frac{1}{K_i^2 K_f^2} \\ & \times \langle 0 | [\exp(-i\mathbf{K}_f \cdot \mathbf{r}) - 1] [\exp(i\mathbf{K}_i \cdot \mathbf{r}) - 1] | 0 \rangle \end{aligned} \quad (19.202)$$

with  $\mathbf{K}_i = \mathbf{k}_i - \mathbf{k}$  and  $\mathbf{K}_f = \mathbf{k}_f - \mathbf{k}$ . The matrix elements in eq. (19.202) may now be readily evaluated and the remaining integration on  $\mathbf{k}$  can be carried out by means of the Feynman parametrization technique used in Section 8.6 and described in detail in Appendix D. As a refinement of the above procedure one may also include exactly a certain number of low-lying states in the sum on  $n$  appearing in eq. (19.200), and then perform the sum on the remaining states by using closure. Since the ground state  $|0\rangle$  lies well below the cluster of other bound states near the continuum, it is reasonable to include this state exactly. In what follows we shall call  $\bar{f}_{\text{B2}}$  the approximate second Born term obtained in this way. Thus we have

$$\begin{aligned} \bar{f}_{\text{B2}} = & \frac{2}{\pi^2} \int d\mathbf{k} \frac{1}{\kappa^2 - k'^2 - i\epsilon} \frac{1}{K_i^2 K_f^2} \\ & \langle 0 | [\exp(-i\mathbf{K}_f \cdot \mathbf{r}) - 1] [\exp(i\mathbf{K}_i \cdot \mathbf{r}) - 1] | 0 \rangle \\ & + \frac{2}{\pi^2} \int d\mathbf{k} \frac{1}{\kappa^2 - k^2 - i\epsilon} \frac{1}{K_i^2 K_f^2} \\ & \times \langle 0 | [\exp(-i\mathbf{K}_f \cdot \mathbf{r}) - 1] | 0 \rangle \langle 0 | [\exp(i\mathbf{K}_i \cdot \mathbf{r}) - 1] | 0 \rangle \\ & - \frac{2}{\pi^2} \int d\mathbf{k} \frac{1}{\kappa^2 - k'^2 - i\epsilon} \frac{1}{K_i^2 K_f^2} \\ & \times \langle 0 | [\exp(-i\mathbf{K}_f \cdot \mathbf{r}) - 1] | 0 \rangle \langle 0 | [\exp(i\mathbf{K}_i \cdot \mathbf{r}) - 1] | 0 \rangle. \end{aligned} \quad (19.203)$$

Of particular interest is the limit of the expression  $\bar{f}_{\text{B2}}$  for large values of  $k$ . It may be shown [53] that at small scattering angles ( $\theta < 2\bar{w}/k^2$ ),  $\text{Re } \bar{f}_{\text{B2}}$  varies like  $k^{-1}$  while  $\text{Im } \bar{f}_{\text{B2}}$  behaves like  $k^{-1} \log k$ . We note that this behaviour of  $\bar{f}_{\text{B2}}$  is quite different from that found in Section 8.6 for the case of potential scattering. In particular, we remark that  $\text{Re } \bar{f}_{\text{B2}}$ , when combined with  $\bar{f}_{\text{B1}}$ , now gives the *dominant correction* to the first Born differential cross section at small momentum transfers. For intermediate momentum transfers



(such that  $k^{-1} \lesssim \Delta \simeq 1$ ) one has  $\text{Re } \tilde{f}_{B2} \sim k^{-2}$  and  $\text{Im } \tilde{f}_{B2} \sim k^{-1}$ . Finally, at large momentum transfers (such that  $\Delta \gtrsim k$ ) one has  $\text{Re } \tilde{f}_{B2} \sim k^{-2} \Delta^{-2}$  and  $\text{Im } \tilde{f}_{B2} \sim k^{-1} \Delta^{-2} \log \Delta$ , a behaviour characteristic of the scattering by the static potential (19.158).

Let us now consider the Glauber elastic scattering amplitude (19.118), together with the associated multiple scattering series defined by eqs. (19.120)–(19.121). We recall that if the Glauber phase shift function (19.119) is evaluated with the  $z$ -axis perpendicular to the momentum transfer  $\Delta$ , we have exactly  $\tilde{f}_{G1} = \tilde{f}_{B1}$  for all scattering angles.

In order to compare the higher terms of the Born series (19.196) and the Glauber series (19.120), we first note that for the interaction potential (19.133c) the Glauber phase shift function (19.119) is given by

$$\chi_{\text{tot}}^G(\mathbf{b}_0, \mathbf{b}_1) = \frac{1}{k} \log \left[ 1 - 2 \frac{b_1}{b_0} \cos(\phi_1 - \phi_0) + \frac{b_1^2}{b_0^2} \right] \quad (19.204)$$

where  $\phi_i$  ( $i = 0, 1$ ) is the azimuthal angle of  $\mathbf{b}_i$  in the  $(x, y)$  plane. Similarly, for a target atom with  $Z$  electrons,

$$\chi_{\text{tot}}^G(\mathbf{b}_0, \mathbf{b}_1, \dots, \mathbf{b}_Z) = \frac{1}{k} \sum_{j=1}^Z \log \left[ 1 - 2 \frac{b_j}{b_0} \cos(\phi_j - \phi_0) + \frac{b_j^2}{b_0^2} \right]. \quad (19.205)$$

Since  $\chi_{\text{tot}}^G$  only depends on the differences  $(\phi_j - \phi_0)$  it is obvious that we may choose the  $x$ - and  $y$ -axis so that no  $\phi_0$  dependence appears in  $\chi_{\text{tot}}^G$ . Hence eq. (19.118) yields

$$f_{e1}^G = \frac{k}{i} \int_0^\infty db_0 b_0 J_0(\Delta b_0) \langle 0 | [\exp(i\chi_{\text{tot}}^G) - 1] | 0 \rangle \quad (19.206)$$

and similarly, we see from eq. (19.121) that

$$\tilde{f}_{Gn} = \frac{k}{i} \frac{i^n}{n!} \int_0^\infty db_0 b_0 J_0(\Delta b_0) \langle 0 | [\chi_{\text{tot}}^G]^n | 0 \rangle. \quad (19.207)$$

It is apparent from eq. (19.207) that, as in the case of potential scattering (see Section 9.1) the terms of the Glauber multiple scattering series (19.120) are alternatively purely real and purely imaginary. This, again, is in contrast to the Born series (19.196), where already the term  $\tilde{f}_{B2}$  contains a real and an imaginary part. A careful analysis of  $\tilde{f}_{G2}$  shows that this term, which is purely imaginary, diverges logarithmically as a function of  $\Delta$  (the length of the momentum transfer) when  $\Delta$  tends to zero [55]. However, although the quantities  $\text{Im } \tilde{f}_{B2}$  and  $\text{Im } \tilde{f}_{G2}$  differ substantially at *very small momentum transfers* because of the divergence of  $\text{Im } \tilde{f}_{G2}$  at  $\Delta = 0$ , a detailed study of these two quantities [53] shows that otherwise they agree very well, even in the backward direction and for rather low values of  $k$ . As an example, we show in Fig. 19.6 the values of  $\text{Im } \tilde{f}_{B2}$  and  $\text{Im } \tilde{f}_{G2}$  as a function of  $\Delta$  for elastic electron–hydrogen scattering at an energy of 100 eV. The agreement between the two quantities is seen to be excellent.

For  $n \geq 3$ , the terms  $\tilde{f}_{Gn}$  of the Glauber multiple scattering series (19.120) are finite, even at  $\Delta = 0$ . It is therefore very plausible that these terms will agree with the corresponding ones of the Born series (i.e.  $\tilde{f}_{G3}$  with  $\text{Re } \tilde{f}_{B3}$ ,  $\tilde{f}_{G4}$  with  $i \text{Im } \tilde{f}_{B4}$ , etc. . . .) when  $k$  is sufficiently large. Since it is extremely difficult to evaluate the quantity  $\text{Re } \tilde{f}_{B3}$  (which yields contributions of order  $k^{-2}$  to the differential cross section) it is therefore reasonable to use  $\tilde{f}_{G3}$  in place of  $\text{Re } \tilde{f}_{B3}$ . Thus we write the *direct* elastic scattering amplitude (through terms of order  $k^{-2}$ ) as

$$f_{el}^d = \tilde{f}_{B1} + \text{Re } \tilde{f}_{B2} + \tilde{f}_{G3} + i \text{Im } \tilde{f}_{B2}. \quad (19.208)$$

In what follows we shall call this expression the *eikonal-Born series* (EBS) approximation for  $f_{el}^d$ .

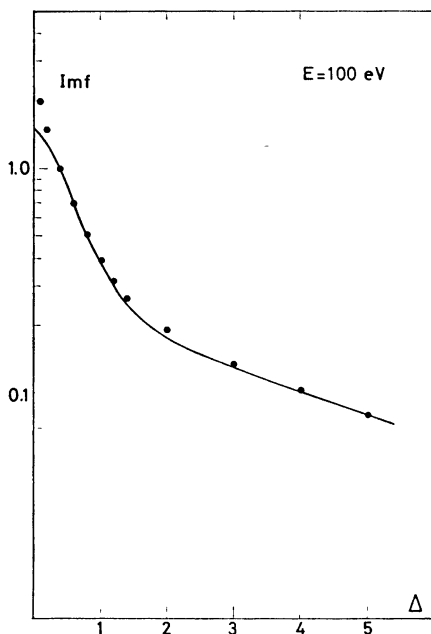


Fig. 19.6. Comparison of the quantities  $\text{Im } \tilde{f}_{B2}$  (solid curve) and  $\text{Im } \tilde{f}_{G2}$  (dots), as a function of the magnitude  $\Delta$  of the momentum transfer, for elastic scattering of 100 eV electrons from the ground state of atomic hydrogen. The average excitation energy  $\bar{\omega}$  used in obtaining  $\text{Im } \tilde{f}_{B2}$  is  $\bar{\omega} = 0.5$  a.u. (taken from ref. [53]).

Before we compute the elastic differential cross section we recall that the leading term of the elastic *exchange* amplitude (i.e. the *Ochkur* term  $g_{el}^{Och}$ ) is of order  $k^{-2}$  for large  $k$  and fixed  $\Delta$  [see eq. (19.191)]. A consistent calculation of the small angle elastic differential cross section through order  $k^{-2}$  therefore requires the inclusion of this term. Hence, for an unpolarized

electron beam and hydrogen atom target, and if no attempt is made to distinguish between the various final spin states, we find with the help of eq. (19.148) that the *eikonal Born series* small angle differential cross section is given through order  $k^{-2}$  by

$$\frac{d\sigma_{el}}{d\Omega} = \frac{1}{4}|f_{el}^d + g_{el}^{Och}|^2 + \frac{3}{4}|f_{el}^d - g_{el}^{Och}|^2 \quad (19.209)$$

where  $f_{el}^d$  is given by eq. (19.208) and  $g_{el}^{Och}$  by eq. (19.191).

The situation at *large momentum transfers* and large  $k$  (i.e. when  $\Delta \gtrsim k$ ) is different. In this limit, the scattering amplitude is dominated by processes in which the atom remains in its ground state in all intermediate states [56, 57]. For example, it is straightforward to verify that the terms  $\text{Re } \tilde{f}_{B2}$  and  $\text{Im } \tilde{f}_{B2}$  are dominated at large momentum transfers by the contribution arising from the ground state  $|0\rangle$  acting as an intermediate state. A detailed study of higher terms of the Born and Glauber series [56, 57], using asymptotic techniques [58], yields similar conclusions. The central role of the ground state in large angle multiple scattering confirms the expectation that high energy, large angle elastic electron-atom scattering is mainly governed by the static potential  $V_{st} = \langle 0|V_d|0\rangle$  [see the discussion following eq. (19.158)].

It is important to remark that for a given (large) value of  $k$ , the convergence of the Born series for the scattering amplitude at large momentum transfers is *slower* than at small momentum transfers. Indeed, it is adversely affected relative to the convergence at small momentum transfers by the presence of powers of  $\log \Delta$  [57]. It is also worth noting that the Ochkur term  $g_{el}^{Och}$ , which behaves like  $k^{-2}\Delta^{-4}$  for large  $\Delta$ , drops off like  $k^{-6}$  when  $\Delta \gtrsim k$ .

In order to illustrate the above discussion, we show in Figs. 19.7 and 19.8 the differential cross sections corresponding to the elastic scattering of electrons by the ground state of atomic hydrogen, at incident electron energies of 50 eV and 100 eV. We display in Fig. 19.7 the curve obtained from the EBS expression (19.209), together with the results obtained by solving numerically the partial wave radial equations corresponding to the static potential (19.158). Also shown on Fig. 19.7 are the first Born values and the Glauber differential cross section

$$d\sigma_{el}^G/d\Omega = |f_{el}^G|^2 \quad (19.210)$$

where the Glauber (direct) elastic amplitude  $f_{el}^G$  is obtained from eq. (19.206). We note from this figure that the EBS results agree reasonably well with the experimental data [59] in spite of the fact that an incident electron energy of 50 eV (corresponding to a wave number  $k \simeq 2$ ) is rather low for the applicability of the EBS method. As we expect, the static results are fairly accurate at large angles, but fail to account for the scattering at small angles, where absorption and polarization effects are important [60]. The first Born results are quite poor, especially at small angles. This is not surprising since the

first Born approximation corresponds precisely to a first order treatment of the static potential  $V_{st}$  [61]. Finally, the Glauber results are seen to be inaccurate over the whole angular range. We recall in this connection that the Glauber differential cross section diverges at  $\theta = 0^\circ$  (because of the term  $\text{Im } \tilde{f}_{G2}$ ) and lacks the exchange term together with the important term  $\text{Re } \tilde{f}_{B2}$  (which, as we have seen above, yields the dominant correction to  $\tilde{f}_{B1}$  at small angles).

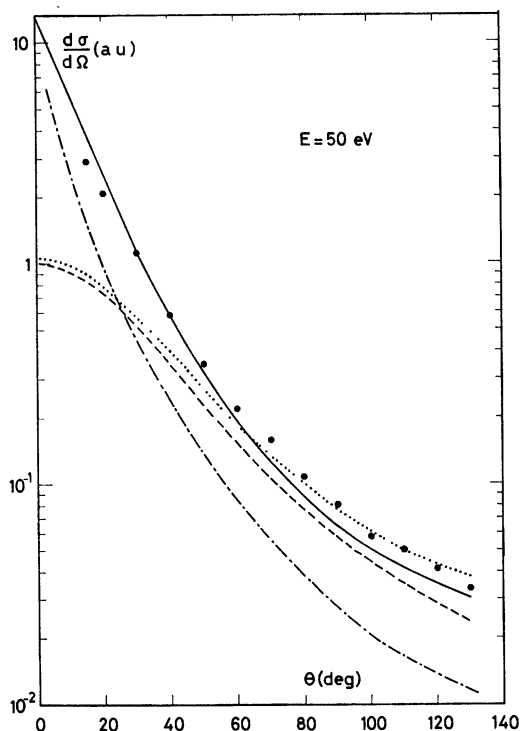


Fig. 19.7. Differential cross section for elastic scattering of electrons by atomic hydrogen at an energy of 50 eV. The solid curve is obtained by using the eikonal-Born series (EBS) method [53, 57]. The dashed curve represents the first Born approximation and the dash-dot curve corresponds to the Glauber approximation. The dotted curve represents the results obtained from a partial wave analysis of the static potential  $V_{st} = \langle 0 | V_d | 0 \rangle$  corresponding to the hydrogen ground state. The dots are the experimental points of ref. [59].

A similar comparison is made in Fig. 19.8 for the elastic scattering of electrons having an energy of 100 eV, at angles  $\theta < 50^\circ$ . Here we have shown the EBS results [obtained from eq. (19.209)] together with the first Born and the Glauber values. We also display in Fig. 19.8 the EBS results corresponding to *positron*-hydrogen elastic scattering. Whereas the eikonal-Born series method predicts significant differences between small angle electron and positron scattering, the Born and Glauber approximation do not distinguish

between the two cases. Also shown in Fig. 19.8 are relative (electron) experimental data [62], normalized to the EBS curve at  $\theta = 30^\circ$ .

We now consider briefly some *inelastic* transitions induced in atomic hydrogen by the impact of fast electrons. Although the eikonal-Born series method discussed above may be generalized to deal with such transitions (at least in simple cases), no calculations of this kind have yet been reported. Instead, one may use for example the less accurate, but simpler *distorted wave Born approximation* (DWBA) of Section 17.4. The basic expression to be evaluated is then the DWBA transition matrix element (17.54), in which the distorted waves  $\chi_a^{(+)}$  and  $\chi_b^{(-)}$  describe respectively the elastic scattering in the initial and final channels. *Eikonal* DWBA calculations for the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  transitions, in which the distorted waves  $\chi_a^{(+)}$  and  $\chi_b^{(-)}$  are obtained in the eikonal approximation, have been performed recently [63, 64]. Glauber-type calculations using eq. (19.103) [65] or the more general expression (19.117) [66] have also been carried out for several inelastic transitions induced in atomic hydrogen by fast electrons.

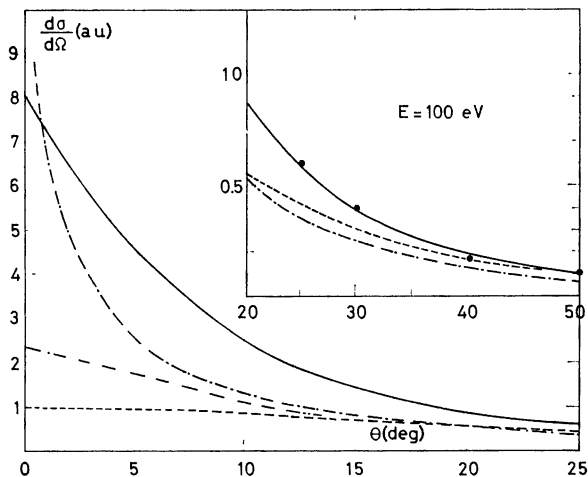


Fig. 19.8. Differential cross section for elastic scattering of electrons and positrons by atomic hydrogen at an energy of 100 eV. The solid curve is obtained for electrons by using the eikonal-Born series (EBS) method of ref. [53]. The dash-double dot curve is the corresponding EBS curve for incident positrons. The dashed curve represents the first Born approximation, and the dash-dot curve corresponds to the Glauber approximation. The experimental points are those of Ref. [62].

#### 19.5.4. Low-energy electron-atomic hydrogen scattering

Among the various methods which have been proposed to analyze low-energy electron-hydrogen scattering [67], a particularly useful one is the *Hulthén-Kohn* variational method which we have described in Section 10.1 for the case of potential scattering.

We begin by recalling the Schrödinger equation for the spatial part of the full wave function. That is,

$$(H - E)\psi^S(\mathbf{r}_0, \mathbf{r}_1) = 0 \quad (19.211a)$$

or

$$\left(-\frac{1}{2}\nabla_{\mathbf{r}_0}^2 - \frac{1}{2}\nabla_{\mathbf{r}_1}^2 - \frac{1}{r_0} - \frac{1}{r_1} + \frac{1}{r_{01}} - E\right)\psi^S(\mathbf{r}_0, \mathbf{r}_1) = 0. \quad (19.211b)$$

Here the subscript  $S$  refers to singlet ( $S = 0$ ) or triplet ( $S = 1$ ) states, and

$$\psi^S(\mathbf{r}_0, \mathbf{r}_1) = (-1)^S \psi^S(\mathbf{r}_1, \mathbf{r}_0). \quad (19.212)$$

Let us consider the simple case of elastic collisions occurring below the first excitation threshold of the hydrogen atom (i.e. for incident electron energies lower than 10.2 eV). Then the phase shifts  $\delta_l^S$  are real and the discussion of Section 10.1.1 can be extended in a straightforward way. For example, in the case of s-wave ( $l = 0$ ) scattering one finds that

$$\left[\frac{\tan \delta_0^S}{k}\right] = \frac{\tan \delta_0^S}{k} + 2 \int \psi_0^S(\mathbf{r}_0, \mathbf{r}_1)(E - H)\psi_0^S(\mathbf{r}_0, \mathbf{r}_1) d\mathbf{r}_0 d\mathbf{r}_1 \quad (19.213)$$

where the s-wave trial wave function  $\psi_0^S$  has the asymptotic form

$$\begin{aligned} \psi_0^S(\mathbf{r}_0, \mathbf{r}_1) \xrightarrow[r_1 \rightarrow \infty]{r_0 \rightarrow \infty} & \{1 + (-1)^S P_{01}\} \left\{ \psi_0(r_1) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{4\pi}} \right. \\ & \left. \times (kr_0)^{-1} (\sin kr_0 + \tan \delta_0^S \cos kr_0) \right\}. \end{aligned} \quad (19.214)$$

Here  $\psi_0(r_1) = \pi^{-1/2} \exp(-r_1)$  is the ground state wave function of the hydrogen atom and  $P_{01}$  is an operator which interchanges the coordinates  $\mathbf{r}_0$  and  $\mathbf{r}_1$  of the two electrons.

Schwartz [68] has made a detailed analysis of this problem. He used trial functions of the form [see eqs. (10.39)–(10.40)]

$$\psi_0^S = \phi^S + \sum_{i=1}^N c_i \chi_i^S \quad (19.215)$$

where the function  $\phi^S$  ensures the correct asymptotic behaviour of  $\psi_0^S$ , the coefficients  $c_i$  are (linear) variational parameters and  $\chi_i^S$  are basis functions. The explicit choice made by Schwartz is

$$\begin{aligned} \phi^S = & \{1 + (-1)^S P_{01}\} \left\{ \psi_0(r_1) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{4\pi}} (kr_0)^{-1} \right. \\ & \left. \times (\sin kr_0 + \tan \delta_0^S \cos kr_0 [1 - \exp(-\frac{1}{2}kr_0)]) \right\} \end{aligned} \quad (19.216)$$

and

$$\chi_i^S \equiv \chi_{j,m,n}^S = \exp\{-\frac{1}{2}\kappa(r_0 + r_1)\} r_{01}^j (r_0^m r_1^n + (-1)^S r_0^n r_1^m). \quad (19.217)$$

The additional (non linear) parameter  $\kappa$  is a scale factor to be varied at the end of the calculations. The choice (19.217) of functions  $\chi_{j,m,n}^S$  is based on the experience gained in performing variational calculations for bound states of two-electron systems. The basis functions  $\chi_{j,m,n}^S$  are ordered in such a way that one always uses all functions with  $j + m + n \leq N$  and then increases  $N$ .

For a given value of the scale factor  $\kappa$ , the problem reduces to a simple one of matrix inversion. By using the method described in Section 10.1 to extract the "average" value of  $\tan \delta_0^S$  between the singularities (see Fig. 10.1), Schwartz has obtained accurate value of the singlet and triplet s-wave phase shifts  $\delta_0^{S=0}$  and  $\delta_0^{S=1}$ . Table 19.1 summarizes some of his results, obtained for various values of the wave number  $k$ . At zero energy he found very accurate values of the singlet and triplet *scattering lengths*, namely  $\alpha(S=0) = 5.965 \pm 0.003$  and  $\alpha(S=1) = 1.7686 \pm 0.0002$  (in a.u.).

TABLE 19.1  
Singlet ( $S=0$ ) and triplet ( $S=1$ ) s-wave phase shifts for elastic electron-hydrogen scattering, obtained by Schwartz [68] from the Hulthén-Kohn variational method

$k$ (a.u.)	$\delta_0^{S=0}$ (radians)	$\delta_0^{S=1}$ (radians)
0.1	2.553	2.939
0.2	2.067	2.717
0.3	1.696	2.500
0.4	1.415	2.294
0.5	1.202	2.105

The Hulthén-Kohn variational principle (10.53) for the *scattering amplitude*, obtained in Section 10.1 for potential scattering, can also be generalized to deal with the present case. It may be used to derive various approximation methods for low-energy electron-atom scattering [67]. Of particular importance is the *close-coupling* method [69] which may be obtained from the (generalized) Hulthén-Kohn variational principle by using trial functions of the form

$$\psi^S(\mathbf{r}_0, \mathbf{r}_1) = \{1 + (-1)^S P_{01}\} \sum_{n=0}^N F_n(\mathbf{r}_0) \psi_n(\mathbf{r}_1) \quad (19.218)$$

where the hydrogenic wave functions  $\psi_n(\mathbf{r}_1)$ , corresponding to the eigenvalues  $w_n$ , satisfy the Schrödinger equation

$$\left( -\frac{1}{2} \nabla_{\mathbf{r}_1}^2 - \frac{1}{r_1} - w_n \right) \psi_n(\mathbf{r}_1) = 0. \quad (19.219)$$

In principle the sum on  $n$  appearing in eq. (19.218) should include both discrete and continuum states of the hydrogen atom, but owing to the difficulties in dealing with the continuum the standard close coupling method only includes a few *discrete* hydrogen states in the sum. Even with this simplifying assumption the equations (obtained from the generalized Hulthén–Kohn variational principle) which determine the unknown functions  $F_n(\mathbf{r}_0)$  are integro-differential equations [70] whose solution require modern computing techniques. The close-coupling method, which can also be used above the first inelastic threshold, has been applied successfully to a variety of low-energy electron–atom scattering processes. Other useful low-energy approximations include the method of “polarized orbitals” and the “non-adiabatic” approach developed by Temkin et al. [71]. A detailed discussion of these methods is given in reference [67], where a comprehensive account of low-energy electron–atom scattering may be found.

### 19.6. High-energy hadron–deuteron scattering

A long-standing problem of great interest, hadron–deuteron scattering at high energies has recently attracted considerable interest, both theoretical and experimental. Lying on the borderline between elementary particle physics and nuclear physics, hadron–deuteron scattering has been a source of fruitful interaction between the two fields. In this section we shall give an introduction to hadron–deuteron collisions within the framework of the Glauber theory discussed in Section 19.4. More complete reviews of high-energy hadron–deuteron scattering may be found in the references [32, 41, 72].

Let us denote by  $\mathbf{r}_n$  and  $\mathbf{r}_p$  the coordinates of the neutron and the proton in the deuteron so that the internal relative vector of the deuteron is  $\mathbf{r}_d = \mathbf{r}_p - \mathbf{r}_n$ . The scattering amplitude for a collision in which the deuteron is in a final state  $|f\rangle$  and the incident particle transferred a momentum  $\hbar\mathbf{q} = \hbar(\mathbf{k}_L - \mathbf{k}_L')$  to the deuteron is then given in the laboratory system by eq. (19.110), with

$$\Gamma_{\text{tot}} = 1 - \exp\{i[\chi_n(\mathbf{b} - \tfrac{1}{2}\mathbf{s}) + \chi_p(\mathbf{b} + \tfrac{1}{2}\mathbf{s})]\}. \quad (19.220)$$

The quantities  $\chi_n$  and  $\chi_p$  are the phase shifts contributed respectively by the neutron and the proton, while the vector  $\mathbf{s}$  is the projection of the relative vector  $\mathbf{r}_d$  of the deuteron in the plane of impact parameters. If we define the objects

$$\Gamma_n(\mathbf{b}) = 1 - \exp\{i\chi_n(\mathbf{b})\} \quad (19.221a)$$

and

$$\Gamma_p(\mathbf{b}) = 1 - \exp\{i\chi_p(\mathbf{b})\} \quad (19.221b)$$

we may write eq. (19.220) as

$$\Gamma_{\text{tot}} = \Gamma_n(\mathbf{b} - \tfrac{1}{2}\mathbf{s}) + \Gamma_p(\mathbf{b} + \tfrac{1}{2}\mathbf{s}) - \Gamma_n(\mathbf{b} - \tfrac{1}{2}\mathbf{s})\Gamma_p(\mathbf{b} + \tfrac{1}{2}\mathbf{s}) \quad (19.222)$$



leading to the physical interpretation in terms of single and double scattering, as we expect from the discussion following eq. (19.113). To analyze this situation in more detail, we note that the functions  $\Gamma_n$  and  $\Gamma_p$  can be expressed in terms of hadron-nucleon laboratory scattering amplitudes  $f_n$  and  $f_p$  by an approximate two-dimensional Fourier inversion. Indeed, if we write eq. (19.102) in the laboratory system, multiply by  $\exp(-i\mathbf{q} \cdot \mathbf{b}')$  and integrate on the variable  $\mathbf{q}$  over a plane perpendicular to the  $z$ -direction, we find that

$$\begin{aligned} \int d^2\mathbf{q} \exp(-i\mathbf{q} \cdot \mathbf{b}') f(\mathbf{q}) &= \frac{ik_L}{2\pi} \int d^2\mathbf{q} \int d^2\mathbf{b} \exp\{i\mathbf{q} \cdot (\mathbf{b} - \mathbf{b}')\} \Gamma(\mathbf{b}) \\ &= 2\pi ik_L \int d^2\mathbf{b} \delta(\mathbf{b} - \mathbf{b}') \Gamma(\mathbf{b}) \end{aligned}$$

so that

$$\Gamma(\mathbf{b}) = (2\pi ik_L)^{-1} \int d^2\mathbf{q} \exp(-i\mathbf{q} \cdot \mathbf{b}) f(\mathbf{q}). \quad (19.223)$$

We note that the accuracy of eq. (19.223) depends on the fact that the scattering is focused in the forward direction, in which case the difference between integrating over a plane or over a sphere (which more accurately corresponds to the locus of momentum transfers for fixed energy) is negligible

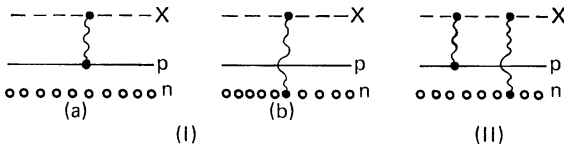


Fig. 19.9. The two types of diagrams which contribute to elastic hadron-deuteron scattering in the high-energy diffraction theory (I) (a) and (b): *single* scattering diagrams; (II) *double* scattering diagram. In those diagrams a solid line represents a proton, a dotted line a neutron and a dashed line the incident hadron X.

Returning to eqs. (19.110) and (19.222) and using eq. (19.223) we find that

$$\begin{aligned} f_{m0}^G &= \left\langle m \left| \exp(i\frac{1}{2}\mathbf{q} \cdot \mathbf{s}) f_n(\mathbf{q}) + \exp(-i\frac{1}{2}\mathbf{q} \cdot \mathbf{s}) f_p(\mathbf{q}) \right. \right. \\ &\quad \left. \left. + \frac{i}{2\pi k_L} \int d^2\mathbf{q}' \exp(i\mathbf{q}' \cdot \mathbf{s}) f_n(\mathbf{q}' + \frac{1}{2}\mathbf{q}) f_p(-\mathbf{q}' + \frac{1}{2}\mathbf{q}) \right| 0 \right\rangle \quad (19.224) \end{aligned}$$

a formula which clearly justifies the interpretation of the collision in terms of single and double scattering processes. The two types of diagrams which contribute to the scattering are shown in Fig. 19.9. The first two terms on the right of eq. (19.224), corresponding to the two first diagrams I(a) and I(b) of Fig. 19.9, give the single scattering or *impulse approximation* contribution to the scattering amplitude  $f_{m0}^G$ . The next term is the double scattering correction.

As a particular case of eq. (19.224), let us first examine the scattering amplitude for *elastic* hadron–deuteron scattering, namely

$$f_{\text{el}}^G = \left\langle 0 \left| \left\{ \exp(i\frac{1}{2}\mathbf{q} \cdot \mathbf{s}) f_n(\mathbf{q}) + \exp(-i\frac{1}{2}\mathbf{q} \cdot \mathbf{s}) f_p(\mathbf{q}) \right. \right. \right. \\ \left. \left. \left. + \frac{i}{2\pi k_L} \int d^2\mathbf{q}' \exp(i\mathbf{q}' \cdot \mathbf{s}) f_n(\mathbf{q}' + \frac{1}{2}\mathbf{q}) f_p(-\mathbf{q}' + \frac{1}{2}\mathbf{q}) \right\} \right| 0 \right\rangle. \quad (19.225)$$

If we denote by  $\psi_0(\mathbf{r}_d)$  the ground state deuteron wave function, we see that we must evaluate integrals of the form

$$S(\mathbf{q}) = \int \exp(i\mathbf{q} \cdot \mathbf{s}) |\psi_0(\mathbf{r}_d)|^2 d\mathbf{r}_d. \quad (19.226)$$

Since the vector  $\mathbf{s}$  is the component of the vector  $\mathbf{r}_d$  which lies in the “impact parameter” plane, and since the momentum transfer vector  $\mathbf{q}$  also lies in this plane (provided we neglect its longitudinal component  $q_z$ ) we see that the quantity  $S(\mathbf{q})$  may be written as

$$S(\mathbf{q}) = \int \exp(i\mathbf{q} \cdot \mathbf{r}_d) |\psi_0(\mathbf{r}_d)|^2 d\mathbf{r}_d. \quad (19.227)$$

In general, an expression such as  $S(\mathbf{q})$ , which is proportional to the Fourier transform of the bound state probability density  $|\psi_0|^2$  is known as the *form factor* of the bound state  $|0\rangle$ . The quantity  $S(\mathbf{q})$  given by eq. (19.227) is therefore the form factor of the deuteron ground state. In terms of this expression we may now write eq. (19.225) as

$$f_{\text{el}}^G(\mathbf{q}) = f_n(\mathbf{q}) S(\frac{1}{2}\mathbf{q}) + f_p(\mathbf{q}) S(-\frac{1}{2}\mathbf{q}) \\ + \frac{i}{2\pi k_L} \int S(\mathbf{q}') f_n(\frac{1}{2}\mathbf{q} + \mathbf{q}') f_p(\frac{1}{2}\mathbf{q} - \mathbf{q}') d^2\mathbf{q}'. \quad (19.228)$$

As a first useful application of eq. (19.228), let us calculate the total hadron–deuteron cross section by using the optical theorem. We write

$$\sigma_{\text{tot}}^d = \frac{4\pi}{k_L} \text{Im } f_{\text{el}}^G(q = 0) \quad (19.229)$$

and we also note that the total hadron–neutron and hadron–proton cross sections are given by

$$\sigma_{\text{tot}}^j = \frac{4\pi}{k_L} \text{Im } f_j(q = 0), \quad j = n, p. \quad (19.230)$$

Moreover, since  $S(q = 0) = 1$ , we deduce from eq. (19.228) that

$$\sigma_{\text{tot}}^d = \sigma_{\text{tot}}^n + \sigma_{\text{tot}}^p - \delta\sigma \quad (19.231)$$

where  $\delta\sigma$ , the “cross section defect”, is given by

$$\delta\sigma = -\frac{2}{k_L^2} \operatorname{Re} \left\{ \int S(\mathbf{q}) [f_n(\mathbf{q}) f_p(-\mathbf{q})] d^2\mathbf{q} \right\}. \quad (19.232)$$

If the size of the deuteron is much larger than the range of the hadron-nucleon interaction, we may write approximately

$$\delta\sigma \simeq -\frac{2}{k_L^2} \operatorname{Re} [f_n(0) f_p(0)] \int S(\mathbf{q}) d^2\mathbf{q}. \quad (19.233)$$

Now, using eq. (19.227), we have

$$\int S(\mathbf{q}) d^2\mathbf{q} = \int d\mathbf{r}_d |\psi_0(\mathbf{r}_d)|^2 \int d^2\mathbf{q} \exp(i\mathbf{q} \cdot \mathbf{r}_d) = 2\pi \langle r_d^{-2} \rangle \quad (19.234)$$

where, for a spherically symmetric ground state wave function

$$\langle r_d^{-2} \rangle = \langle \psi_0 | r_d^{-2} | \psi_0 \rangle = 4\pi \int_0^\infty dr_d |\psi_0(r_d)|^2. \quad (19.235)$$

Hence, eq. (19.233) becomes

$$\delta\sigma \simeq -\frac{4\pi}{k_L^2} \operatorname{Re} [f_n(0) f_p(0)] \langle r_d^{-2} \rangle.$$

Furthermore, if we assume that the amplitudes  $f_n(0)$  and  $f_p(0)$  are purely imaginary – so that the nucleons are “black” – we obtain the very simple approximate result

$$\delta\sigma \simeq \frac{1}{4\pi} \sigma_{\text{tot}}^n \sigma_{\text{tot}}^p \langle r_d^{-2} \rangle \quad (19.236)$$

where we have used again eq. (19.230).

A variety of other interesting cross sections may be derived from eqs (19.224) and (19.225). The elastic differential cross section is given by

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{el}} = |f_{\text{el}}^G|^2. \quad (19.237)$$

The total scattered intensity is obtained from

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{sc}} = \sum_m |f_{m0}^G|^2 \quad (19.238)$$

and can be evaluated by using the closure relation on the deuteron final states. Inelastic processes in which the deuteron is dissociated in two free nucleons are calculated from

$$\left( \frac{d\sigma}{d\Omega} \right)_{\text{in}} = \left( \frac{d\sigma}{d\Omega} \right)_{\text{sc}} - \left( \frac{d\sigma}{d\Omega} \right)_{\text{el}}. \quad (19.239)$$

The corresponding total cross sections  $\sigma_{el}$ ,  $\sigma_{sc}$  and  $\sigma_{in} = \sigma_{sc} - \sigma_{el}$  are directly obtained by integrating eqs. (19.237)–(19.239) over the angles. Finally, the “absorption” cross section

$$\sigma_{abs} = \sigma_{tot}^d - \sigma_{sc} \quad (19.240)$$

corresponds to all processes where the incident hadron disappears during the collision or reappears with one or several produced particles [73].

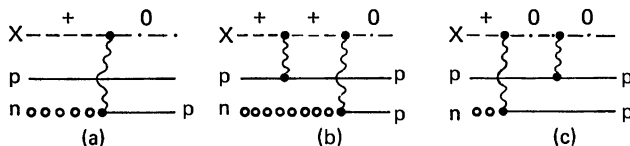


Fig. 19.10. The various processes which contribute to charge-exchange scattering by the deuteron in the case of a positively charged (+) incident hadron of isotopic spin  $\frac{1}{2}$ . The dash-dot line (with index 0) denotes the corresponding neutral hadron.

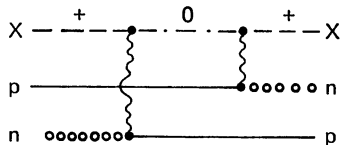


Fig. 19.11. The double charge-exchange process.

The generalization of these considerations to include the spin and isospin degrees of freedom of the incident particle and the target nucleons has been carried out by several authors [42, 74–77]. For example, the single and double collision diagrams contributing to charge-exchange scattering by the deuteron in the case of an incident hadron of isotopic spin  $\frac{1}{2}$  are represented in Fig. 19.10 whereas in Fig. 19.11 the double charge-exchange process leading to no net transfer of charge is displayed. In particular, this last effect may be shown to yield a small correction to the cross section defect  $\delta\sigma$  obtained in eq. (19.232). The result is [75]

$$\delta\sigma = -\frac{2}{k_L^2} \operatorname{Re} \left\{ \int S(\mathbf{q}) \frac{1}{2} [f_p(\mathbf{q})f_n(-\mathbf{q}) + f_n(\mathbf{q})f_p(-\mathbf{q}) - f_c(\mathbf{q})f_c(-\mathbf{q})] d^2\mathbf{q} \right\} \quad (19.241)$$

where  $f_c(\mathbf{q})$  is the charge-exchange amplitude. The three terms of this expression correspond to the three possibilities of elastic double scattering processes. The first two terms describe charge-preserving collisions with both the neutron and the proton in the two possible orders. The third term corresponds to the

double charge-exchange process. If the hadron–nucleon force range is small compared with the size of the deuteron, we may write again

$$\delta\sigma \simeq -\frac{4\pi}{k_L^2} \text{Re}\{f_n(0)f_p(0) - \frac{1}{2}[f_n(0) - f_p(0)]^2\} \langle r_d^{-2} \rangle \quad (19.242)$$

a formula which under the assumption of purely imaginary amplitudes  $f_n(0)$  and  $f_p(0)$  reduces to [compare with eq. (19.236)]

$$\delta\sigma \simeq \frac{1}{4\pi} [\sigma_{\text{tot}}^n \sigma_{\text{tot}}^p - \frac{1}{2}(\sigma_{\text{tot}}^n - \sigma_{\text{tot}}^p)^2] \langle r_d^{-2} \rangle. \quad (19.243)$$

Franco and Glauber [42] have applied the theory described above to analyze antiproton–deuteron collisions in the GeV range. They assume that at high energies the antiproton–nucleon scattering amplitudes  $f_{\bar{p}N}$  are such that (we are using here a more explicit notation for the individual two-body amplitudes)

$$f_{\bar{p}N}(q) = f_{\bar{p}p}(q) = f_{\bar{p}n}(q)$$

and may be parametrized as

$$f_{\bar{p}N} = i(k_L \sigma_{\bar{p}N}/4\pi) \exp(-\beta q^2)$$

where  $\sigma_{\bar{p}N}$  is the total antiproton–nucleon cross section and  $\beta$  is a parameter determined from the experimental data on (two-body) antiproton–nucleon scattering. The total and absorption antiproton–deuteron cross sections obtained by Franco and Glauber are shown respectively in Figs. 19.12 and 19.13. They exhibit an appreciable double scattering effect.

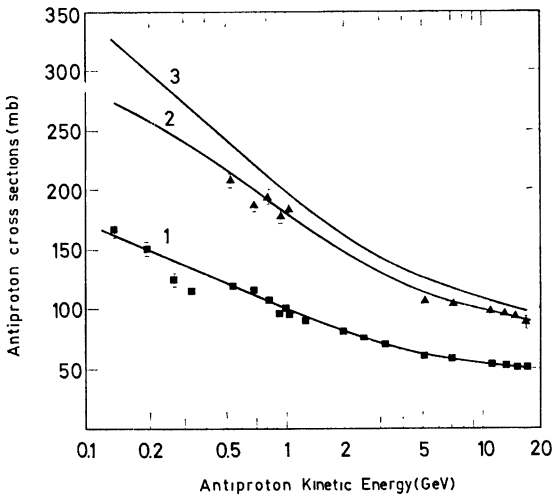


Fig. 19.12. Total cross sections for antiproton–proton and antiproton–deuteron collisions, as a function of the antiproton laboratory kinetic energy. Curve 1 is a fit to the experimental values of the total antiproton–proton cross section. Curve 2 corresponds to the antiproton–deuteron total cross section calculated by Franco and Glauber [42]. Curve 3 represents twice the antiproton–proton total cross section. The total cross section defect is the difference between the ordinate of curves 3 and 2 (taken from ref. [42]).

We now turn to a more detailed analysis of the angular distribution of elastic hadron-deuteron scattering, with particular attention to proton-deuteron scattering [78]. We first note that the double scattering term appearing in eq. (19.228) tends to counteract the effect of the two single scattering terms. In fact, if the amplitudes  $f_{pn}$  and  $f_{pp}$  (we use again a more explicit

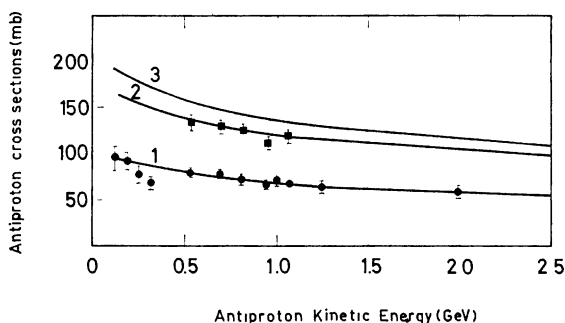


Fig. 19.13. Absorption cross sections for antiproton-proton and antiproton-deuteron collisions, as a function of the incident antiproton laboratory kinetic energy. Curve 1 is a fit to the experimental values of the antiproton-proton absorption cross section. Curve 2 represents the deuteron absorption cross section as obtained by Franco and Glauber [42]. Curve 3 gives twice the antiproton-proton absorption cross section. The cross section defect for absorption is the difference between the ordinates of curves 3 and 2 (taken from ref. [42]).

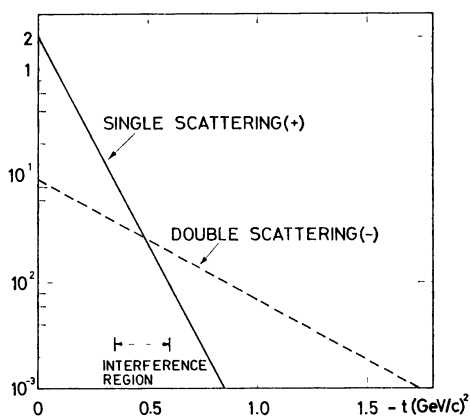


Fig. 19.14. The contributions to the amplitude ratio  $f_{pd}(-t)/f_{pN}(0)$  from the single and double scattering terms corresponding to the elastic scattering of 20 GeV/c protons by deuterons (taken from ref. [41]).

notation) were purely imaginary, a simple calculation shows that the double scattering term would completely cancel the contribution of the single scattering amplitudes at  $-t \simeq 0.5 (\text{GeV}/c)^2$ , where the Mandelstam variable  $t$  is the square of the four-momentum transfer of the collision (see Section 2.2).

The contribution of the single and double scattering terms for such a parametrization of the amplitude  $f_{pN}$  (where  $N$  denotes a nucleon) is shown in Fig. 19.14. It is seen that the single scattering terms dominate near the forward direction. At larger momentum transfers the double scattering term, which decreases more slowly [79] with increasing  $q$ , becomes the dominant contribution to the scattering amplitude  $f_{e1}^G$ .

Let us now consider more closely the intermediate region of momentum transfers, where the single and double scattering terms interfere destructively.

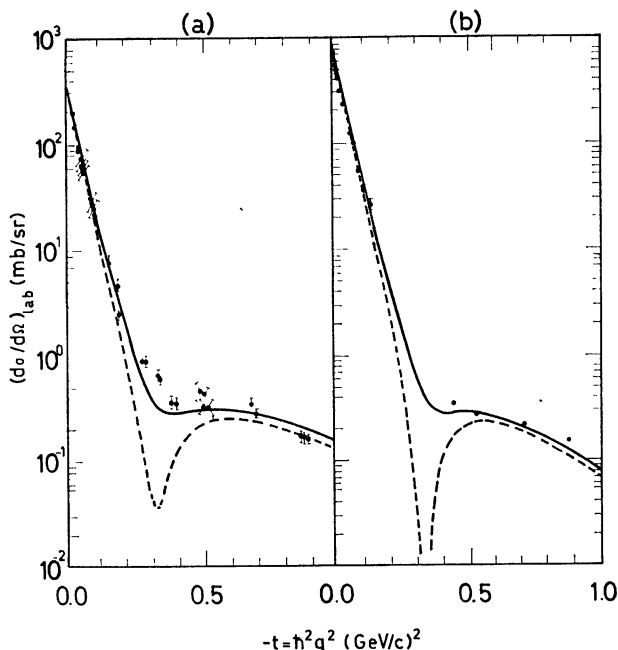


Fig. 19.15. Differential cross sections corresponding to the elastic scattering of (a) 1-GeV and (b) 2-GeV protons by unpolarized deuterons. *Dashed curve*: results obtained by including only the S-state of the deuteron. *Solid curve*: calculations including both S and D states of the deuteron. The dots refer to the experimental data. (Taken from Franco and Glauber [81].)

This region is therefore of special interest, since it depends delicately upon the phases of the hadron-nucleon amplitudes. Moreover, as shown in Fig. 19.15, this interference region is very sensitive to the choice of the ground state wave function of the deuteron. It is only by including the quadrupole deformation of the deuteron, i.e. by taking into account the D-state part of the deuteron wave function [80] that Franco and Glauber [81] found good agreement with the experimental data on proton-deuteron elastic scattering at 1 and 2 GeV [82, 83]. Similar conclusions hold for high-energy pion-deuteron scattering [77, 84, 85].

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$$\langle q|V|q_i\rangle = (2\pi)^{-3} \int d\mathbf{r} d\mathbf{r}' \exp(-i\mathbf{q}'\cdot\mathbf{r}) \langle r|V|r'\rangle \exp(i\mathbf{q}\cdot\mathbf{r}'). \quad (19.24)$$
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$$[K] \equiv \begin{pmatrix} 0 & T_1 G_0 & T_1 G_0 \\ T_2 G_0 & 0 & T_2 G_0 \\ T_3 G_0 & T_3 G_0 & 0 \end{pmatrix}.$$
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requires the evaluation of the expression  $\langle n | \sum_{j=1}^Z \exp(i\mathbf{d} \cdot \mathbf{r}_j) | 0 \rangle$ . The related quantity

$$f_{n0}(\Delta) = \frac{2(w_n - w_0)}{\Delta^2} |\langle n | \sum_{j=1}^Z \exp(i\Delta z_j) | 0 \rangle|^2$$

– which enters into the calculation of first Born cross sections – is called the *generalized oscillator strength* corresponding to the transition  $0 \rightarrow n$ .

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$$\sigma_{\text{tot}}^{2p,1s} \simeq 576\pi \left(\frac{2}{3}\right)^{1/2} \frac{1}{k^2} \left[ \log(4k_i) - \frac{137}{120} \right]. \quad (19.181')$$

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## The Optical Potential

In this chapter we want to study the *elastic* scattering of a given particle by a composite target containing several scatterers. Such processes are conveniently analyzed by replacing the very complicated interactions between the beam and target particles by an *optical potential* – or *pseudopotential* – in which the incident particle moves. Once the optical potential is determined, the original many-body elastic scattering problem reduces to a one-body problem, namely the scattering of a particle by a potential. However, as we shall see in what follows, the price of reducing a many-body problem to a one-body situation is that the optical potential will in general be a complicated non-local, complex operator whose determination from first principles is often difficult to achieve. Thus for practical applications we shall require approximation methods to determine the optical potential.

As one should expect from the terminology, the earliest application of the optical model method was made in the field of optics, in particular to the analysis of the propagation of light through a refractive medium. In this case, the use of a complex refractive index is in fact equivalent to the introduction of an optical potential [1]. An early generalization of the optical model ideas was made by Ostrofsky, Breit and Johnson [2] to the study of  $\alpha$ -decay of nuclei, while Bethe [3] introduced the concept of an optical potential in order to describe low-energy nuclear reactions within the “compound nucleus” model. The description of high-energy nuclear collisions by means of the optical model formalism was initiated by Serber *et al.* [4], who first tried to describe elastic nucleon–nucleus scattering in terms of nucleon–nucleon collisions. They argued that at high energies nuclear collisions should proceed by way of collisions with individual target nucleons. Using known nucleon–nucleon cross sections, this multiple scattering analysis led to the conclusion

that particles should move more or less freely through nuclear matter at high energies (partial “transparency” of nuclei). This fact was verified qualitatively by experiment, and led to a reassessment of the optical model for low-energy nuclear scattering [5].

Following the work of Serber *et al.*, several attempts were made to explore the foundations of the optical model and to obtain it from the many-body Schrödinger equation. After showing in Section 20.1 how an optical potential may be introduced to describe elastic scattering, we discuss in Section 20.2 the formal derivations of Watson *et al.* [6–8], of Glauber [9] and of Feshbach [10]. As we shall see, the formal expressions obtained in this way are quite complicated, and may only be explicitly evaluated in simple cases. One of these is high-energy elastic hadron–nucleus scattering, which we shall discuss in detail in Section 20.3. Another case for which useful approximations may be devised to obtain the optical potential is the elastic scattering of charged particles by atoms. This problem will be treated in Section 20.4 [11].

## 20.1. Elastic scattering and the optical potential

In this section we first show how the elastic scattering of a particle from a composite target may be described in terms of an optical potential. We then explore the consequences of the optical theorem in order to extract various cross sections from our knowledge of the elastic scattering amplitude in the forward direction.

### 20.1.1 Introduction of the optical potential

Let us consider the elastic scattering of an “elementary” incident particle by a target made up of  $N$  scatterers. We denote by  $M$  and  $S$  the mass and spin of the incident particle, by  $k$  and  $k'$  its initial and final wave vectors and by  $v$  and  $v'$  its initial and final spin orientations. The wave functions of the incident particle, before and after the scattering event, are then given by

$$\Phi_{i,k,v} = (2\pi)^{-3/2} \exp(ik \cdot r_i) \chi_{S,v}(s_i) \quad (20.1a)$$

and

$$\Phi_{i,k',v'} = (2\pi)^{-3/2} \exp(ik' \cdot r_i) \chi_{S,v'}(s_i) \quad (20.1b)$$

where  $r_i$  and  $s_i$  are respectively the space and spin coordinates and the subscript  $i$  refers to the incident particle. If  $K_i$  denotes the kinetic energy operator of the incident particle, we have

$$K_i \Phi_{i,k,v} = E(k) \Phi_{i,k,v} \quad (20.2a)$$

and

$$K_i \Phi_{i,k',v'} = E(k') \Phi_{i,k',v'} \quad (20.2b)$$

where  $E(k)$  and  $E(k')$  are respectively the initial and final energies of the "beam" particle. Thus for a non-relativistic incident particle, we have

$$E(k) = \hbar^2 k^2 / 2M \quad (20.3)$$

while

$$E(k) = c\sqrt{M^2 c^2 + \hbar^2 k^2} \quad (20.4)$$

for a relativistic beam particle.

We have assumed that the target is composed of  $N$  elementary scatterers. We call  $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$  their spatial coordinates and  $s_1, s_2, \dots, s_N$  their spin coordinates. The total mass of the target is denoted by  $M_t$  and its angular momentum by  $S_t$ . We also call  $\mathbf{K}$  and  $\mathbf{K}'$  the initial and final total wave vectors of the target while  $\mathbf{v}_t$  and  $\mathbf{v}'_t$  are its initial and final spin orientations. If  $\psi_{0, \mathbf{v}_t}(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N)$  and  $\psi_{0, \mathbf{v}'_t}$  denote the internal bound state wave function of the target before and after the collision, we may write the complete target wave function, before and after elastic scattering [12] as

$$\Phi_{t, \mathbf{K}, 0, \mathbf{v}_t} = (2\pi)^{-3/2} \exp(i\mathbf{K} \cdot \mathbf{R}) \psi_{0, \mathbf{v}_t}(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N) \quad (20.5a)$$

and

$$\Phi_{t, \mathbf{K}', 0, \mathbf{v}'_t} = (2\pi)^{-3/2} \exp(i\mathbf{K}' \cdot \mathbf{R}) \psi_{0, \mathbf{v}'_t}(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N). \quad (20.5b)$$

Here the subscript  $t$  indicates that we are dealing with the target system, whose center of mass coordinate is called  $\mathbf{R}$ . The Hamiltonian for the target is given by

$$h_t = \sum_{j=1}^N K_j + U \quad (20.6)$$

where  $K_j$  is the kinetic energy operator for particle  $j$  and  $U$  is the interaction between the  $N$  particles of the target. In what follows we shall assume that the target may be described by a non-relativistic Hamiltonian  $h_t$ . We shall then write

$$h_t = K_{t, \text{c.m.}} + h \quad (20.7)$$

where the center of mass kinetic energy operator of the target is given in the coordinate representation by

$$K_{t, \text{c.m.}} = -\frac{\hbar^2}{2M_t} \nabla_{\mathbf{R}}^2 \quad (20.8)$$

and  $h$  is the internal target Hamiltonian, with eigenvalues  $w_n$  (the internal target energies) and eigenvectors  $\psi_n$  such that

$$h\psi_n = w_n\psi_n. \quad (20.9)$$

The wave function  $\psi_0$  which describes the internal state of the target, before and after the elastic scattering, evidently belongs to the set  $\{\psi_n\}$  and is such that  $h\psi_0 = w_0\psi_0$ . In what follows we shall assume that the wave function

$\psi_0$  is known, if only approximately. In many important applications, where the elastic scattering proceeds from the *ground* state of the target, powerful methods are indeed available to determine [13] the wave function  $\psi_0$ . Returning to the target Hamiltonian (20.6) and using eq. (20.7) we may now write

$$h_t \Phi_{t,K,0,v_t} = W_0 \Phi_{t,K,0,v_t} \quad (20.10a)$$

and

$$h_t \Phi_{t,K',0,v'_t} = W'_0 \Phi_{t,K',0,v'_t} \quad (20.10b)$$

where

$$W_0 = w_0 + \hbar^2 K^2 / 2M_t \quad (20.11a)$$

and

$$W'_0 = w_0 + \hbar^2 K'^2 / 2M_t. \quad (20.11b)$$

Consider now the system made up of the incident particle and the target. The motion of the system in the asymptotic region before the collision (i.e. without interaction between the incident particle and the target) is governed by the Hamiltonian

$$H_d = K_i + h_t. \quad (20.12)$$

In accordance with the definitions adopted in Chapter 14 we have used the subscript *d* to indicate that the arrangement channel Hamiltonian  $H_d$  corresponds to *direct* scattering. We note that since the target is a bound state of  $N$  scatterers the Hamiltonian  $H_d$  differs from the Hamiltonian  $H_0$  corresponding to  $(N + 1)$  free particles. We also have

$$H_d \Phi_a = E_a \Phi_a, \quad (20.13a)$$

$$H_d \Phi_b = E_b \Phi_b. \quad (20.13b)$$

Here

$$\Phi_a = \Phi_{i,k,v} \Phi_{t,K,0,v_t} \quad (20.14a)$$

and

$$\Phi_b = \Phi_{i,k',v'} \Phi_{t,K',0,v'_t} \quad (20.14b)$$

are the initial and final asymptotic states of the target plus incident particle and

$$E_a = E(k) + W_0 = E(k) + w_0 + \hbar^2 K^2 / 2M_t, \quad (20.15a)$$

$$E_b = E(k') + W'_0 = E(k') + w_0 + \hbar^2 K'^2 / 2M_t \quad (20.15b)$$

where we have used eqs. (20.11). Conservation of energy yields the relation  $E_a = E_b$ , or

$$E(k) + \hbar^2 K^2 / 2M_t = E(k') + \hbar^2 K'^2 / 2M_t. \quad (20.16)$$

The Hamiltonian for the entire system, including the interaction  $V_d$  between the incident particle and the target, is given by

$$H = H_d + V_d \quad (20.17)$$

where

$$V_d = \sum_{j=1}^N v_j \quad (20.18)$$

is the sum of all the interactions  $v_j$  between the beam particle and the  $j$ th target scatterer.

Because no internal degrees of freedom are excited during an elastic scattering process, we may consider it as formally equivalent to the potential scattering of two particles having no structure. Following Watson *et al.* [8, 11] we shall call  $\mathcal{T}_c$  the corresponding transition operator. The index  $c$  refers to coherent (or elastic) scattering. A typical matrix element of  $\mathcal{T}_c$  is therefore given by

$$\langle \mathbf{k}', v', \mathbf{K}', v'_i | \mathcal{T}_c | \mathbf{k}, v, \mathbf{K}, v_i \rangle \equiv \langle \mathbf{k}', v', \mathbf{K}', 0, v'_i | \mathcal{T} | \mathbf{k}, v, \mathbf{K}, 0, v_i \rangle \quad (20.19a)$$

where  $\mathcal{T}$  is the complete transition operator. The submatrix of  $\mathcal{T}_c$  defined on the momentum shell  $(\mathbf{k} + \mathbf{K} = \mathbf{k}' + \mathbf{K}')$  will be denoted by  $T_c$ . Hence [14]

$$\begin{aligned} \langle \mathbf{k}', v', \mathbf{K}', v'_i | \mathcal{T}_c | \mathbf{k}, v, \mathbf{K}, v_i \rangle \\ = \delta(\mathbf{k}' + \mathbf{K}' - \mathbf{k} - \mathbf{K}) \langle \mathbf{k}', v', \mathbf{K}', v'_i | T_c | \mathbf{k}, v, \mathbf{K}, v_i \rangle. \end{aligned} \quad (20.19b)$$

According to the discussion of Section 15.2 the differential cross section for a particular elastic scattering process  $(\mathbf{k}, v, \mathbf{K}, v_i) \rightarrow (\mathbf{k}', v', \mathbf{K}', v'_i)$  is given by

$$\begin{aligned} \frac{d\sigma_{el}}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \int d\mathbf{k}' k'^2 \delta \left( E(k') + \frac{\hbar^2 K'^2}{2M_t} - E(k) - \frac{\hbar^2 K^2}{2M_t} \right) \\ \times |\langle \mathbf{k}', v', \mathbf{K}', v'_i | T_c | \mathbf{k}, v, \mathbf{K}, v_i \rangle|^2 \end{aligned} \quad (20.20)$$

where  $v_i$  is the initial relative velocity. For a random distribution of the initial spin orientations of the incident particle and the target, and if we do not detect the final spin orientations, the corresponding differential elastic cross section  $d\bar{\sigma}_{el}/d\Omega$  must be summed over the final spin orientations and averaged over the initial ones, in which case we obtain

$$\frac{d\bar{\sigma}_{el}}{d\Omega} = \frac{1}{(2S+1)(2S_t+1)} \sum_{v_i, v'_i} \frac{d\sigma_{el}}{d\Omega}. \quad (20.21)$$

Since the elastic scattering is formally identical to a simple two-body scattering problem, it is reasonable to introduce an *optical potential* or *pseudopotential*  $\mathcal{V}_{opt}$  such that [compare with eqs. (16.21)]

$$\mathcal{T}_c = \mathcal{V}_{opt} + \mathcal{V}_{opt} \frac{1}{E(k) + \hbar^2 K^2/2M_t - E(p) - \hbar^2 P^2/2M_t + i\varepsilon} \mathcal{T}_c. \quad (20.22a)$$

Here  $p$  and  $P$  are intermediate (virtual) momenta of the incident particle and of the center of mass of the target. We may also write eq. (20.22a) in the alternative form

$$\mathcal{T}_c(E_a) = \mathcal{V}_{opt} + \mathcal{V}_{opt} \frac{1}{E_a - H_d + i\varepsilon} \mathcal{T}_c(E_a) \quad (20.22b)$$



if we agree to extend the definition of  $\mathcal{T}_e$  by including a projection operator onto the states  $\psi_{0,v_i}$ . Thus the optical potential  $\mathcal{V}_{\text{opt}}$  is defined as an operator which, through the Lippmann–Schwinger equations (20.22) leads to the exact transition matrix  $\mathcal{T}_e$  corresponding to the elastic scattering of the incident particle by the target. It is clear from eqs. (20.22) that  $\mathcal{V}_{\text{opt}}$  is also a  $(2S+1)(2S_i+1) \times (2S+1)(2S_i+1)$  matrix in spin space, having matrix elements of the form

$$\langle \mathbf{k}', v', K', v_i | \mathcal{V}_{\text{opt}} | \mathbf{k}, v, K, v_i \rangle = \delta(\mathbf{k}' + \mathbf{K}' - \mathbf{k} - \mathbf{K}) \langle \mathbf{k}', v', K', v_i | V_{\text{opt}} | \mathbf{k}, v, K, v_i \rangle \quad (20.23)$$

where  $V_{\text{opt}}$  is the sub-matrix of  $\mathcal{V}_{\text{opt}}$  defined on the momentum shell.

It is important to note that until now we have made no particular choice of a coordinate system. If we elect to work in the *center of mass system*, we may eliminate from the preceding formulae the variables related to the (overall) center of mass of the entire system. In this case the total Hamiltonian is still given by

$$H = H_d + V_d$$

where the interaction  $V_d$  is always obtained from eq. (20.18). However, the “unperturbed” Hamiltonian  $H_d$  is now such that

$$H_d = K + h \quad (20.24)$$

where  $h$  is the internal target Hamiltonian and  $K$  is the relative kinetic energy operator. For example, if this relative motion is non-relativistic, we have in the coordinate representation

$$K = -\frac{\hbar^2}{2m} \nabla_r^2 \quad (20.25)$$

where  $m = MM_i/(M + M_i)$  is the reduced mass of the colliding particles and where  $\mathbf{r} = \mathbf{r}_i - \mathbf{R}$  is the relative vector joining the position of the

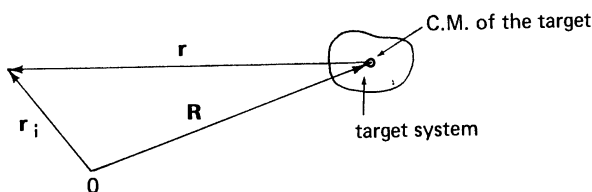


Fig. 20.1. Illustration of the vectors  $\mathbf{r}_i$ ,  $\mathbf{R}$  and  $\mathbf{r}$  of the text.

center of mass of the target to that of the incident particle (see Fig. 20.1). The initial and final free states satisfying eqs. (20.13) are then given by

$$\Phi_a = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \chi_{S,v} \psi_{0,v_i} \quad (20.26a)$$

and

$$\Phi_b = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}) \chi_{S,v} \psi_{0,v_i} \quad (20.26b)$$

where  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are respectively the *relative* initial and final wave vectors. We note that since the coordinate of the (overall) center of mass has been eliminated, the free states  $\Phi_a$  and  $\Phi_b$ , expressed in the position representation, will depend only on  $N$  relative spatial coordinates, namely the vector  $\mathbf{r}$  together with  $(N - 1)$  relative vectors appearing in  $\psi_{0,v_i}$  (or  $\psi_{0,v_f}$ ). If we denote by  $E(k_i)$  and  $E(k_f)$  the relative kinetic energies in the initial and final states, the total energy available in the C.M. system before the collision is given by

$$E_a = E(k_i) + w_0, \quad k_i = |\mathbf{k}_i| \quad (20.27a)$$

while after the elastic scattering we have

$$E_b = E(k_f) + w_0, \quad k_f = |\mathbf{k}_f|. \quad (20.27b)$$

For a non-relativistic relative motion we have

$$E(k_i) = \hbar^2 k_i^2 / 2m, \quad E(k_f) = \hbar^2 k_f^2 / 2m \quad (20.28)$$

where  $m$  is the reduced mass introduced in eq. (20.25). For a relativistic relative motion we have instead

$$\begin{aligned} E(k_i) &= c[\sqrt{M^2 c^2 + \hbar^2 k_i^2} + \sqrt{M_t^2 c^2 + \hbar^2 k_i^2}], \\ E(k_f) &= c[\sqrt{M^2 c^2 + \hbar^2 k_f^2} + \sqrt{M_t^2 c^2 + \hbar^2 k_f^2}]. \end{aligned} \quad (20.29)$$

Conservation of energy in the C.M. system implies from eqs. (20.27) that  $E(k_i) = E(k_f)$ , so that  $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ .

The matrices  $T_c$  and  $V_{\text{opt}}$ , defined on the momentum shell, are also conveniently expressed in the C.M. system. We then have to consider matrix elements of the form

$$\langle \mathbf{k}_f, v', v'_i | T_c | \mathbf{k}_i, v, v_i \rangle$$

or

$$\langle \mathbf{k}_f, v', v'_i | V_{\text{opt}} | \mathbf{k}_i, v, v_i \rangle$$

and eq. (20.22a) becomes

$$T_c = V_{\text{opt}} + V_{\text{opt}} \frac{1}{A} T_c. \quad (20.30)$$

Here we have set

$$A \equiv E(k_i) + \frac{\hbar^2 k_i^2}{2M_t} - E(\kappa) - \frac{\hbar^2 \kappa^2}{2M_t} + i\epsilon \quad (20.31)$$

and  $\kappa$  is an intermediate wave vector in the C.M. system. If the incident particle motion is non-relativistic we have  $E(k_i) = \hbar^2 k_i^2 / 2m$  in which case we may write the quantity  $A$  as

$$A = \frac{\hbar^2 k_i^2}{2m} - \frac{\hbar^2 \kappa^2}{2m} + i\epsilon \quad (20.32)$$

where  $m$  is the reduced mass introduced in eq. (20.25).

As in Section 15.2 we may perform the integration appearing in eq. (20.20) to obtain the C.M. differential cross section for an elastic scattering process of the type  $(\mathbf{k}_i, v, v_i) \rightarrow (\mathbf{k}_f, v', v'_i)$ . The result is

$$\frac{d\sigma_{el}}{d\Omega} = \frac{(2\pi)^4}{\hbar v_i} \rho_b(E) |\langle \mathbf{k}_f, v', v'_i | T_c | \mathbf{k}_i, v, v_i \rangle|^2 \quad (20.33)$$

where  $E = E_a = E_b$  and [see eq. (15.46)]

$$\rho_b(E) = km/\hbar^2 \quad (20.34)$$

for a non-relativistic collision. In the relativistic case one has [see eq. (15.39)]

$$\rho_b(E) = \frac{k}{\hbar^2 c^2 (1/E_i + 1/E_t)} \quad (20.35)$$

where  $E_i$  and  $E_t$  are respectively the (relativistic) energies of the “incident” and “target” particles in the C.M. system. For a random distribution of initial spins and if the final spin orientations are undetected the averaged C.M. differential cross section  $d\bar{\sigma}_{el}/d\Omega$  is of course obtained by substituting in eq. (20.21) the value of  $d\sigma_{el}/d\Omega$  evaluated from eq. (20.33).

We now turn to an important question, namely: “How is the optical potential  $\mathcal{V}_{opt}$  related to the many-body problem?” In order to investigate this point, we first consider the many-body scattering wave function  $\Psi_a^{(+)}$ , solution of the Lippmann–Schwinger equation

$$\Psi_a^{(+)} = \Phi_a + \frac{1}{E_a - H_d + i\varepsilon} V_d \Psi_a^{(+)} \quad (20.36)$$

The wave function  $\Psi_a^{(+)}$  evidently describes both the elastic and non-elastic scattering. Since we are particularly interested in the description of elastic collisions we call  $\Psi_{c,a}^{(+)}$  that part of  $\Psi_a^{(+)}$  corresponding to coherent (elastic) scattering, and write

$$\Psi_{c,a}^{(+)} = \Pi_0 \Psi_a^{(+)} \quad (20.37)$$

where

$$\Pi_0 = \sum_{v'_i} \psi_{0,v'_i} \psi_{0,v'_i}^\dagger \equiv \sum_{v'_i} |\psi_{0v'_i}\rangle \langle \psi_{0v'_i}| \quad (20.38)$$

is a projection operator onto the states  $\psi_{0,v_i}$ . From eqs. (16.15) and (20.19) we also deduce that

$$\Psi_{ca}^{(+)} = \Phi_a + \frac{1}{E_a - H_d + i\varepsilon} \mathcal{T}_c \Phi_a \quad (20.39)$$

or, using eqs. (20.22), we find that  $\Psi_{ca}^{(+)}$  satisfies the integral equations

$$\begin{aligned} \Psi_{ca}^{(+)} &= \Phi_a + \frac{1}{E_a - H_d + i\varepsilon} \mathcal{V}_{opt} \Psi_{ca}^{(+)} \\ &= \Phi_a + \frac{1}{E(k) + \hbar^2 K^2/2M_t - E(p) - \hbar^2 P^2/2M_t + i\varepsilon} \mathcal{V}_{opt} \Psi_{ca}^{(+)} \end{aligned} \quad (20.40)$$

These are precisely Lippmann–Schwinger equations involving the optical potential  $\mathcal{V}_{\text{opt}}$ . From eqs. (20.39) and (20.40) we also see that

$$\mathcal{T}_c \Phi_a = \mathcal{V}_{\text{opt}} \Psi_{ca}^{(+)} \quad (20.41)$$

Since we want to reduce the original many-body situation to a two-body problem, it is natural to eliminate the target bound state wave functions from eqs. (20.40). To this end we write eqs. (20.37)–(20.38) as

$$|\Psi_{ca}^{(+)}\rangle = \sum_{v_i'} |\psi_{0,v_i'}\rangle \langle \psi_{0,v_i'} | \Psi_a^{(+)} \rangle$$

or

$$\Psi_{ca}^{(+)} = \sum_{v_i'} \psi_{0,v_i'} \varphi_{k,v,K,v_i}^{(+)} \quad (20.42)$$

where we have retained only the relevant initial channel labels to define

$$\varphi_{k,v,K,v_i}^{(+)} = \langle \psi_{0,v_i'} | \Psi_a^{(+)} \rangle.$$

We note that  $\varphi_{k,v,K,v_i}^{(+)}$  is an object having  $(2S+1)(2S_i+1)$  components in spin space. From eqs. (20.40) and (20.42) we then deduce that the function  $\varphi_{k,v,K,v_i}^{(+)}$  satisfies the Lippmann–Schwinger equation

$$\varphi_{k,v,K,v_i}^{(+)} = \Phi_{k,v,K,v_i} + \frac{1}{E(k) + \hbar^2 K^2 / 2M_t - E(p) - \hbar^2 P^2 / 2M_t + i\varepsilon} \mathcal{V}_{\text{opt}} \varphi_{k,v,K,v_i}^{(+)} \quad (20.43)$$

with

$$\Phi_{k,v,K,v_i} = (2\pi)^{-3} \exp(i\mathbf{k} \cdot \mathbf{r}_i) \exp(i\mathbf{K} \cdot \mathbf{R}) \chi_{v,v_i} \quad (20.44)$$

where  $\chi_{v,v_i}$  is the appropriate spin function for the two spins  $S$  and  $S_i$ , having respectively the orientations  $v$  and  $v_i$ . Eq. (20.43) may be further simplified in the C.M. system, where it becomes

$$\varphi_{k_i,v,v_i}^{(+)} = \Phi_{k_i,v,v_i} + \frac{1}{A} V_{\text{opt}} \varphi_{k_i,v,v_i}^{(+)} \quad (20.45)$$

where  $A$  is given by eq. (20.31) and

$$\Phi_{k_i,v,v_i} = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}) \chi_{v,v_i}. \quad (20.46)$$

From eqs. (20.30) and (20.45) we also deduce that

$$T_c \Phi_{k_i,v,v_i} = V_{\text{opt}} \varphi_{k_i,v,v_i}^{(+)} \quad (20.47)$$

### 20.1.2. The role of the optical theorem

We have defined above the optical potential  $\mathcal{V}_{\text{opt}}$  as the potential leading to the elastic scattering transition matrix  $\mathcal{T}_c$  by means of the Lippmann–Schwinger equations (20.22). This definition does not imply that the optical potential is an Hermitian operator. In fact, as we shall now see, the optical

potential is in general *non-Hermitian*. To show how this comes about, let us examine some of the implications of the unitarity relations, and in particular of the *optical theorem*. Using eqs. (15.175) and (15.176), we write

$$\begin{aligned}\sigma_{\text{tot}} &= \frac{4\pi}{k_i} \text{Im } f_{\text{el}}^0 \\ &= -2 \frac{(2\pi)^3}{\hbar v_i} \text{Im} \langle \mathbf{k}_i, v, v_t | T_c | \mathbf{k}_i, v, v_t \rangle.\end{aligned}\quad (20.48)$$

Here  $\sigma_{\text{tot}}$  is the total (complete) cross section for all scattering processes originating from the initial state  $\Phi_a$  of eq. (20.26a) and all the quantities appearing on the right-hand side of eq. (20.48) are written in the C.M. system.

Let us now write

$$\sigma_{\text{tot}} = \sigma_{\text{tot}}^{\text{el}} + \sigma_{\text{tot}}^{\text{r}} \quad (20.49)$$

where  $\sigma_{\text{tot}}^{\text{el}}$  is the total cross section for all *elastic* scattering processes, while  $\sigma_{\text{tot}}^{\text{r}}$  is the total “reaction” cross section for all *non-elastic* collisions.

Let us first consider the total elastic cross section. By summing over all final states in eq. (20.33) we obtain

$$\sigma_{\text{tot}}^{\text{el}} = \frac{(2\pi)^4}{\hbar v_i} \langle \Phi_\alpha | T_c^\dagger \delta(B) T_c | \Phi_\alpha \rangle \quad (20.50)$$

where  $B = A - i\varepsilon$ ,  $A$  is defined by eq. (20.31) and we have set  $\alpha \equiv (\mathbf{k}_i, v, v_t)$ . We may transform the right-hand side of eq. (20.50) as follows. We first use eq. (11.167) to write

$$\frac{1}{A^\dagger} - \frac{1}{A} = 2\pi i \delta(B).$$

Hence

$$\sigma_{\text{tot}}^{\text{el}} = -\frac{(2\pi)^3}{\hbar v_i} i \left\langle \Phi_\alpha \left| T_c^\dagger \left( \frac{1}{A^\dagger} - \frac{1}{A} \right) T_c \right| \Phi_\alpha \right\rangle. \quad (20.51)$$

Furthermore, using eqs. (20.45) and (20.47), we find that

$$\sigma_{\text{tot}}^{\text{el}} = \frac{(2\pi)^3}{\hbar v_i} i [\langle \Phi_\alpha | T_c^\dagger | \varphi_\alpha^{(+)} \rangle - \langle \varphi_\alpha^{(+)} | T_c | \Phi_\alpha \rangle + \langle \Phi_\alpha | T_c - T_c^\dagger | \Phi_\alpha \rangle]. \quad (20.52)$$

We now return to the optical theorem [eq. (20.48)] which we write as

$$\sigma_{\text{tot}} = -2 \frac{(2\pi)^3}{\hbar v_i} \frac{1}{2i} \langle \Phi_\alpha | T_c - T_c^\dagger | \Phi_\alpha \rangle. \quad (20.53)$$

Thus, after comparison of eqs. (20.49), (20.52) and (20.53), we deduce that

$$\sigma_{\text{tot}}^{\text{r}} = -\frac{(2\pi)^3}{\hbar v_i} i [\langle \Phi_\alpha | T_c^\dagger | \varphi_\alpha^{(+)} \rangle - \langle \varphi_\alpha^{(+)} | T_c | \Phi_\alpha \rangle]$$

or, using again eq. (20.47)

$$\sigma_{\text{tot}}^r = -\frac{(2\pi)^3}{\hbar v_i} i [\langle \varphi_{\alpha}^{(+)} | V_{\text{opt}}^{\dagger} | \varphi_{\alpha}^{(+)} \rangle - \langle \varphi_{\alpha}^{(+)} | V_{\text{opt}} | \varphi_{\alpha}^{(+)} \rangle]$$

so that

$$\sigma_{\text{tot}}^r = -2 \frac{(2\pi)^3}{\hbar v_i} \text{Im} \langle \varphi_{\alpha}^{(+)} | V_{\text{opt}} | \varphi_{\alpha}^{(+)} \rangle. \quad (20.54)$$

We note immediately that the right-hand side of eq. (20.54) would vanish if  $V_{\text{opt}}$  were an Hermitian operator. Conversely, if non-elastic collisions can occur so that  $\sigma_{\text{tot}}^r \neq 0$ , the optical potential must be non-Hermitian. This is a natural consequence of the fact that the colliding system can leave the incident (elastic) channel so that no conservation of probability is required *within the elastic channel* [15].

As an illustration of the considerations developed so far, let us consider a target which is nearly uniform on the scale of the de Broglie wavelength of the incident particle. If the target were very large and *completely* uniform, giving rise to a constant complex value  $V_0$  of  $V_{\text{opt}}$ , we would write (in the C.M. system)

$$\varphi_{\mathbf{k}_i, v_i}^{(+)} = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \chi_{v_i} \quad (20.55)$$

where  $\kappa = |\mathbf{k}|$  is the wave number in the target medium such that

$$E(k_i) = E(\kappa) + V_0. \quad (20.56)$$

But

$$E(\kappa) = E(k_i) + \frac{dE}{dk_i}(\kappa - k_i) + \dots$$

or

$$E(\kappa) = E(k_i) + \hbar v_i(\kappa - k_i) + \dots \quad (20.57)$$

where we have used the fact that

$$v_i = \hbar^{-1} \frac{dE}{dk_i}$$

is the incident velocity. Upon comparison of eqs. (20.56) and (20.57) we see that for a large uniform medium

$$\kappa \simeq k_i - V_0/\hbar v_i. \quad (20.58)$$

We note that the ratio

$$n = \kappa/k_i \quad (20.59)$$

plays a role which is similar to the refractive index of optics. For this reason it is called the *refractive index* of the target. From eqs. (20.58) and (20.59) we see that in a uniform target medium

$$n \simeq 1 - \frac{V_0}{\hbar v_i k_i} \quad (20.60)$$

so that the introduction of a complex potential  $V_0$  corresponds to that of a complex index of refraction  $n$ .

Let us now consider the case of a target which is *nearly* uniform on the scale of the incident wavelength. In this case we may interpret eq. (20.58) as

$$\kappa(\mathbf{r}) \simeq k_1 - \frac{V_{\text{opt}}(\mathbf{r})}{\hbar v_i} \quad (20.61)$$

where  $V_{\text{opt}}(\mathbf{r})$  and  $\kappa(\mathbf{r})$  are slowly varying functions of  $\mathbf{r}$ . We then write eq. (20.55) as

$$\varphi_{\mathbf{k}_i, \mathbf{v}, \mathbf{v}_t}^{(+)} \simeq (2\pi)^{-3/2} \exp \left[ i\mathbf{k}_i \cdot \mathbf{r} - \frac{i}{\hbar v_i} \int_{-\infty}^z V_{\text{opt}}(\mathbf{b}, z') dz' \right] \chi_{\mathbf{v}, \mathbf{v}_t} \quad (20.62)$$

which is precisely the *eikonal* form [16] of  $\varphi_{\mathbf{k}_i, \mathbf{v}, \mathbf{v}_t}^{(+)}$ . Here we have set  $\mathbf{r} = \mathbf{b} + z \hat{\mathbf{k}}_i$  and we have integrated along a straight line parallel to  $\mathbf{k}_i$ .

As an example, let us consider the elastic scattering of a spinless particle by a spinless target simulated by a complex square well. Writing

$$V_{\text{opt}}(r) = \begin{cases} -V_0, & r < a \\ 0, & r > a \end{cases} \quad (20.63)$$

with

$$V_0 = V_R + iV_I, \quad (V_R, V_I > 0) \quad (20.64)$$

we see from eq. (20.62) that

$$\varphi_{\mathbf{k}_i}^{(+)} = (2\pi)^{-3/2} \exp \left[ i\mathbf{k}_i \cdot \mathbf{r} + \frac{iV_R d}{\hbar v_i} - \frac{V_I d}{\hbar v_i} \right] \quad (20.65)$$

where  $d$  is the distance travelled by the particle through the well in order to arrive at the point  $\mathbf{r}$  (see Fig. 20.2). We note from eq. (20.65) that the wave  $\varphi_{\mathbf{k}_i}^{(+)}$  is exponentially attenuated as it proceeds through the target, this

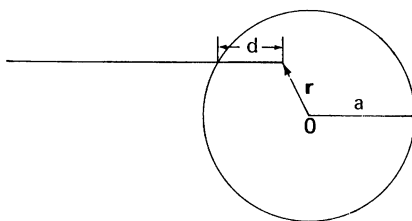


Fig. 20.2. The distances  $a$  and  $d$  and the vector  $\mathbf{r}$  of the text.

attenuation arising from non-elastic collisions which “depopulate” the initial elastic channel. Using eq. (20.54) we may in fact calculate the total “reaction” cross section corresponding to those non-elastic processes. It is given by

$$\sigma_{\text{tot}}^r = \frac{2(2\pi)^3 V_I}{\hbar v_i} \int_{\mathcal{Q}} |\varphi_{\mathbf{k}_i}^{(+)}|^2 d\mathbf{r}$$

or

$$\sigma_{\text{tot}}^r = \frac{1}{A} \int_{\mathcal{Q}} \exp(-d/\Lambda) d\mathbf{r} \quad (20.66)$$

where the domain of integration  $\mathcal{D}$  is a sphere of radius  $a$  and  $\Lambda = \hbar v_i/2V_1$  is the mean free path of the incident particle in the target medium. This integral is readily performed and yields

$$\sigma_{\text{tot}}^r = \pi a^2 \{1 - \frac{1}{2}(\Lambda/a)^2 [1 - (1 + 2a/\Lambda) \exp(-2a/\Lambda)]\}. \quad (20.67)$$

We verify that for very small mean free paths such that  $\Lambda/a \ll 1$  (corresponding to a “black” target) one finds that  $\sigma_{\text{tot}}^r$  reduces to  $\pi a^2$ , which, as expected, is precisely the geometrical cross section of the target.

## 20.2. The optical potential and the many-body problem

We now turn to the problem of deriving the optical potential in terms of the many-body interactions. We shall examine here the formal derivations of Watson *et al.* [6–8], of Glauber [9] and of Feshbach [10].

### 20.2.1. Multiple scattering and the optical potential

Let us assume for the moment that the incident particle is distinct from each of the scatterers in the target. The scattering matrix for elastic scattering may then be written as

$$\mathcal{T}_c = \langle \Phi_b | V_d | \Psi_a^{(+)} \rangle \quad (20.68)$$

where the many-body scattering wave function  $\Psi_a^{(+)}$ , describing both elastic and inelastic scattering satisfies eq. (20.36), the final free state  $\Phi_b$  is obtained from eq. (20.14b) – or eq. (20.26b) in the C.M. system – and  $V_d$ , as given by eq. (20.18) is the full interaction between the incident particle and the target.

Following the method of Watson *et al.*, we introduce an operator  $F$  such that

$$\Psi_a^{(+)} = F \Psi_{ca}^{(+)} \quad (20.69)$$

Thus, in contrast with the projection operator  $\Pi_0$ , the new operator  $F$  “reconstructs” the full many-body wave function from its elastic scattering part. Now, let us operate on both sides of eq. (20.36) with the operator  $\Pi_0$ . Using eq. (20.37), and setting [17]  $G_d^{(+)} = (E_a - H_d + i\varepsilon)^{-1}$ , we obtain

$$\Psi_{ca}^{(+)} = \Phi_a + G_d^{(+)} \mathcal{V}_{\text{opt}} \Psi_{ca}^{(+)} \quad (20.70)$$

with

$$\mathcal{V}_{\text{opt}} \Psi_{ca}^{(+)} = \Pi_0 V_d F \Psi_{ca}^{(+)} \quad (20.71)$$

The optical potential  $\mathcal{V}_{\text{opt}}$  (which does not act on the internal coordinates of the target) is then given by

$$\mathcal{V}_{\text{opt}} = \langle 0 | V_d F | 0 \rangle \quad (20.72)$$

where we have written  $\Pi_0 = |0\rangle\langle 0|$  without explicit spin indices. In order to determine  $\mathcal{V}_{\text{opt}}$  we must therefore find the operator  $F$ . To this end, we start



from eq. (20.36) and write

$$\Psi_a^{(+)} = \Phi_a + G_d^{(+)} V_d \Psi_a^{(+)}$$

or

$$F \Psi_{ca}^{(+)} = \Phi_a + G_d^{(+)} V_d F \Psi_{ca}^{(+)} \quad (20.73)$$

where we have used eq. (20.69) which defines  $F$ . Now, extracting  $\Phi_a$  from eq. (20.70) and substituting in eq. (20.73), we have

$$F \Psi_{ca}^{(+)} = \Psi_{ca}^{(+)} - G_d^{(+)} \mathcal{V}_{\text{opt}} \Psi_{ca}^{(+)} + G_d^{(+)} V_d F \Psi_{ca}^{(+)}. \quad (20.74)$$

The second term on the right-hand side of eq. (20.74) may be modified by using eq. (20.71), so that

$$\begin{aligned} F \Psi_{ca}^{(+)} &= \Psi_{ca}^{(+)} - G_d^{(+)} \Pi_0 V_d F \Psi_{ca}^{(+)} + G_d^{(+)} V_d F \Psi_{ca}^{(+)} \\ &= \{1 + G_d^{(+)}(1 - \Pi_0) V_d F\} \Psi_{ca}^{(+)}. \end{aligned}$$

Hence

$$F = 1 + G_d^{(+)}(1 - \Pi_0) V_d F. \quad (20.75)$$

This is an exact Lippmann–Schwinger equation for  $F$ , which we now proceed to solve approximately. A first, obvious method is to solve eq. (20.75) by successive iterations, starting from  $F = 1$  as our lowest order approximation. In this way we generate for  $F$  a Born series in powers of the interaction  $V_d$ , namely

$$F = 1 + G_d^{(+)}(1 - \Pi_0) V_d + G_d^{(+)}(1 - \Pi_0) V_d G_d^{(+)}(1 - \Pi_0) V_d + \dots \quad (20.76)$$

so that the optical potential  $\mathcal{V}_{\text{opt}}$  is given by

$$\begin{aligned} \mathcal{V}_{\text{opt}} &= \langle 0 | V_d | 0 \rangle + \langle 0 | V_d G_d^{(+)}(1 - \Pi_0) V_d | 0 \rangle \\ &\quad + \langle 0 | V_d G_d^{(+)}(1 - \Pi_0) V_d G_d^{(+)}(1 - \Pi_0) V_d | 0 \rangle + \dots \end{aligned} \quad (20.77)$$

The two first terms of eq. (20.77) will be analyzed in detail in Section 20.4 for the case of the elastic scattering of a charged particle by an atom. We already note here that the first term  $\langle 0 | V_d | 0 \rangle$  is simply the *static potential* of the target (i.e. the full interaction  $V_d$  between the incident particle and the target averaged over the target internal state  $|0\rangle$ ).

A second way of solving eq. (20.75) is to try to express the operator  $F$  in terms of (known) *two-body scattering matrices*. To this end we first define the objects

$$t_j = v_j + v_j G_d^{(+)}(1 - \Pi_0) t_j \quad (20.78)$$

so that the operator  $F$  is given by the *Watson equations*

$$F = 1 + \sum_{j=1}^N G_d^{(+)}(1 - \Pi_0) t_j F_j \quad (20.79a)$$

with

$$F_j = 1 + G_d^{(+)} \sum_{k(\neq j)=1}^N (1 - \Pi_0) t_k F_k. \quad (20.79b)$$

Indeed, substituting eq. (20.79a) into the right-hand side of eq. (20.75), we find that

$$F = 1 + G_d^{(+)}(1 - \Pi_0)V_d + G_d^{(+)}(1 - \Pi_0)V_d G_d^{(+)}(1 - \Pi_0) \sum_{j=1}^N t_j F_j. \quad (20.80)$$

Now, using eqs. (20.18), (20.78) and (20.79b), we have

$$\begin{aligned} \sum_{j=1}^N t_j F_j &= V_d + \sum_{j=1}^N (t_j - v_j) F_j + \sum_{j=1}^N v_j (F_j - 1) \\ &= V_d + \sum_{j=1}^N v_j G_d^{(+)}(1 - \Pi_0) t_j F_j + \sum_{j=1}^N \sum_{k(\neq j)=1}^N v_j G_d^{(+)}(1 - \Pi_0) t_k F_k \\ &= V_d + \sum_{j=1}^N v_j G_d^{(+)}(1 - \Pi_0) \sum_{k=1}^N t_k F_k \end{aligned}$$

so that

$$\sum_{j=1}^N t_j F_j = V_d F \quad (20.81)$$

and eq. (20.80) reduces to

$$\begin{aligned} F &= 1 + G_d^{(+)}(1 - \Pi_0)V_d \{1 + G_d^{(+)}(1 - \Pi_0)V_d F\} \\ &= 1 + G_d^{(+)}(1 - \Pi_0)V_d F \end{aligned} \quad (20.82)$$

which is precisely eq. (20.75). Furthermore, because of eq. (20.81), we also see from eq. (20.72) that the optical potential is given by

$$\mathcal{V}_{\text{opt}} = \left\langle 0 \left| \sum_{j=1}^N t_j F_j \right| 0 \right\rangle. \quad (20.83)$$

This last expression of  $\mathcal{V}_{\text{opt}}$  is an exact one. However, the coupled equations (20.79) are in general very difficult to solve. Indeed, since the Green's operator  $G_d$  involves the target Hamiltonian, the operators  $t_j$ , as defined by eq. (20.78), are still many-body objects.

Let us now assume that the incident particle has high energy with respect to the (absolute value) of any target particle binding energy. In this case the impulse approximation may be used to show that the target particles act mostly as if they were free, so that one may write approximately [18]

$$t_j \simeq \mathcal{T}_j \quad (20.84)$$

where the objects  $\mathcal{T}_j$  are *two-body* transition operators for *free* particles. The Watson equations (20.79) then become

$$F = 1 + G_d^{(+)}(1 - \Pi_0) \sum_{j=1}^N \mathcal{T}_j F_j \quad (20.85a)$$

with

$$F_j = 1 + G_d^{(+)}(1 - \Pi_0) \sum_{k(\neq j)=1}^N \mathcal{T}_k F_k \quad (20.85b)$$

and the optical potential is given by

$$\mathcal{V}_{\text{opt}} = \left\langle 0 \left| \sum_{j=1}^N \mathcal{T}_j F_j \right| 0 \right\rangle. \quad (20.86)$$

Expanding  $F$  as a succession of scatterings, we therefore obtain for  $\mathcal{V}_{\text{opt}}$  the *multiple scattering series*

$$\mathcal{V}_{\text{opt}} = \langle 0 | \sum_{j=1}^N \mathcal{T}_j | 0 \rangle + \langle 0 | \sum_{j=1}^N \sum_{k(\neq j)=1}^N \mathcal{T}_j G_d^{(+)}(1 - \Pi_0) \mathcal{T}_k | 0 \rangle + \cdots \quad (20.87)$$

Until now we have supposed that the incident particle is distinct from each of the target particles. Formal treatments of the scattering of a particle identical with target scatterers have been given by Takeda and Watson [19], Bell and Squires [20] and Feshbach [10]. In particular, Takeda and Watson show that at high energies and when the incident particle is identical with a target particle  $j$  it is only necessary to use the correctly symmetrized (or antisymmetrized) two-body  $\mathcal{T}_j$  in eqs. (20.85)–(20.87).

### 20.2.2 The optical model in the eikonal approximation

The multiple scattering approach to the elastic scattering of a particle by a composite target may also be formulated [9] within the framework of the *eikonal approximation*. Let

$$\mathbf{r} = \mathbf{b} + z\hat{\mathbf{z}}$$

be the relative coordinate and

$$\mathbf{r}_j = \mathbf{b}_j + z_j\hat{\mathbf{z}} \quad (j = 1, 2, \dots, N)$$

be the coordinates of the target particles (with respect to the target center of mass). According to the discussion of Section 9.1 we shall choose the unit vector  $\hat{\mathbf{z}}$  along the bisector of the scattering angle. If the target is initially in the state  $|0\rangle$  and we “freeze” the target scatterers during the passage of the beam particle, we may write the C.M. elastic scattering amplitude in the Glauber eikonal approximation [see eq. (19.118)] as

$$f_{\text{el}}^G = \frac{k}{2\pi i} \int d^2\mathbf{b} \exp(i\mathbf{A} \cdot \mathbf{b}) \langle 0 | [\exp\{i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)\} - 1] | 0 \rangle \quad (20.88)$$

where  $\mathbf{A} = \mathbf{k}_i - \mathbf{k}_f$  is the wave vector transfer in the C.M. system and the Glauber phase shift function  $\chi_{\text{tot}}^G$  is given by

$$\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N) = \sum_{j=1}^N \chi_j(\mathbf{b} - \mathbf{b}_j), \quad (20.89)$$

the quantities  $\chi_j$  being the phase shift functions describing the scattering of the incident particle by each of the target scatterers. Since we want to reduce the original many-body problem to a two-body problem in which the target coordinates have disappeared, it is natural to return to the two-body eikonal amplitude (9.37) [or (19.100)] and to define an optical phase shift function  $\chi_{\text{opt}}$  by the relation

$$f_{\text{el}}^G = \frac{k}{2\pi i} \int d^2\mathbf{b} \exp(i\mathbf{A} \cdot \mathbf{b}) [\exp\{i\chi_{\text{opt}}(\mathbf{b})\} - 1]. \quad (20.90)$$

Provided that recoil effects are neglected, we may also write a similar equation in the laboratory system [see eq. (20.141) below].

Upon comparison of eqs. (20.88) and (20.90), we see that

$$\exp\{i\chi_{\text{opt}}(\mathbf{b})\} = \langle 0 | \exp\{i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)\} | 0 \rangle. \quad (20.91)$$

We note immediately that, except when  $\chi_{\text{tot}}^G$  is independent of the target configuration, we have

$$|\exp(i\chi_{\text{opt}})| \neq 1$$

so that the optical phase shift function  $\chi_{\text{opt}}$  is in general a *complex* quantity. Moreover, if the elementary interactions between the incident particle and the target scatterers are genuine two-body interactions [21] such that the two-body phase shift functions  $\chi_j$  and hence  $\chi_{\text{tot}}$  are *real*, we see that  $\exp(i\chi_{\text{tot}}^G)$  is a unitary operator when acting on the target states  $|n\rangle$ . We then have

$$\sum_n |\langle n | \exp(i\chi_{\text{tot}}^G) | 0 \rangle|^2 = 1$$

or, using eq. (20.91)

$$|\exp(i\chi_{\text{opt}})|^2 + \sum_{n \neq 0} |\langle n | \exp(i\chi_{\text{tot}}^G) | 0 \rangle|^2 = 1. \quad (20.92)$$

Thus

$$|\exp(i\chi_{\text{opt}})| \leq 1 \quad (20.93)$$

and  $\chi_{\text{opt}}$  is real only when  $\chi_{\text{tot}}^G$  is diagonal in the initial target state, i.e. when there is only elastic scattering. As soon as non-elastic transitions occur, the optical phase shift function  $\chi_{\text{opt}}$  acquires a *positive* imaginary part which corresponds to the fact that particles disappear from the elastic scattering channel.

If the “elementary” interactions between the incident particle and the target scatterers must themselves be described in terms of complex phase shift functions  $\chi_j$  having a positive imaginary part [22], then eq. (20.92) becomes

$$|\exp(i\chi_{\text{opt}})|^2 + \sum_{n \neq 0} |\langle n | \exp(i\chi_{\text{tot}}^G) | 0 \rangle|^2 < 1 \quad (20.94)$$

which again implies the fact that  $\chi_{\text{opt}}$  has a positive imaginary part.

Further insight into the optical model may be gained by calculating the optical phase shift function  $\chi_{\text{opt}}$  as a power series in  $\chi_{\text{tot}}^G$ . Following the method of Glauber [9], we write

$$\chi_{\text{opt}}(\mathbf{b}) = -i \log \langle 0 | \exp\{i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_N)\} | 0 \rangle$$

or

$$\chi_{\text{opt}}(\mathbf{b}) = -i \log (1 + i\langle 0 | \chi_{\text{tot}}^G | 0 \rangle - \frac{1}{2}\langle 0 | (\chi_{\text{tot}}^G)^2 | 0 \rangle + \dots)$$

so that

$$\chi_{\text{opt}}(\mathbf{b}) = \langle 0 | \chi_{\text{tot}}^G | 0 \rangle + \frac{1}{2}i\{\langle 0 | (\chi_{\text{tot}}^G)^2 | 0 \rangle - \langle 0 | \chi_{\text{tot}}^G | 0 \rangle^2\} + \dots \quad (20.95)$$

We see from eq. (20.95) that in first order the optical phase shift function  $\chi_{\text{opt}}$  is simply the average of  $\chi_{\text{tot}}^G$  over the target wave function. If the “elementary” interactions between the incident and target particles are described by ordinary real potentials (i.e. by real phase shift functions) and correspond

therefore to genuine two-body problems, we note that the first order term of  $\chi_{\text{opt}}$  is real. In this case an imaginary part of  $\chi_{\text{opt}}$  only appears in second order, and is clearly positive since the quantity in brackets appearing in eq. (20.95) is just the mean variance of the phase shift function.

Let us assume that we have evaluated the optical phase shift function  $\chi_{\text{opt}}$  by means of eq. (20.91) or by using the series (20.95). We may now, within the framework of the eikonal approximation, define an optical potential  $V_{\text{opt}}$  which corresponds to the phase shift function  $\chi_{\text{opt}}$ . It is a *local* operator  $V_{\text{opt}}(\mathbf{r})$  such that

$$\chi_{\text{opt}}(\mathbf{b}) = -\frac{1}{\hbar v_i} \int_{-\infty}^{+\infty} V_{\text{opt}}(\mathbf{b}, z) dz. \quad (20.96)$$

If we assume that  $V_{\text{opt}}$  depends only on  $r = |\mathbf{r}|$ , we have

$$\chi_{\text{opt}}(b) = -\frac{1}{\hbar v_i} \int_{-\infty}^{+\infty} V_{\text{opt}}(\sqrt{b^2 + z^2}) dz \quad (20.97)$$

or

$$\chi_{\text{opt}}(b) = -\frac{2}{\hbar v_i} \int_b^{\infty} \frac{V_{\text{opt}}(r)r dr}{\sqrt{r^2 - b^2}}. \quad (20.98)$$

This last equation is an Abel integral equation which may be solved to yield the optical potential in terms of  $\chi_{\text{opt}}$ . The result is

$$V_{\text{opt}}(r) = \frac{\hbar v_i}{\pi} \frac{1}{r} \frac{d}{dr} \int_r^{\infty} \frac{\chi_{\text{opt}}(b)}{\sqrt{b^2 - r^2}} b db \quad (20.99a)$$

or

$$V_{\text{opt}}(r) = \frac{\hbar v_i}{\pi} \int_r^{\infty} \frac{\chi'_{\text{opt}}(b)}{\sqrt{b^2 - r^2}} db. \quad (20.99b)$$

Having obtained the optical phase shift function  $\chi_{\text{opt}}$  we may compute the elastic scattering amplitude  $f_{\text{el}}^G$  and therefore the corresponding elastic differential cross section. Moreover, since we have reduced the original problem to a two-body problem described by a complex phase shift function  $\chi_{\text{opt}}$ , we may use the formulae (9.54), (9.58) and (9.59) to write respectively the total (complete), total elastic and total non-elastic ("reaction") cross sections as

$$\sigma_{\text{tot}} = 2 \int d^2b [1 - \exp(-\text{Im } \chi_{\text{opt}}) \cos(\text{Re } \chi_{\text{opt}})], \quad (20.100a)$$

$$\sigma_{\text{tot}}^{\text{el}} = \int d^2b |\exp(i\chi_{\text{opt}}) - 1|^2 \quad (20.100b)$$

and

$$\sigma_{\text{tot}}^r = \int d^2b [1 - \exp(-2 \text{Im } \chi_{\text{opt}})] \quad (20.100c)$$

with

$$\chi_{\text{opt}} = \text{Re } \chi_{\text{opt}} + i \text{Im } \chi_{\text{opt}}, \quad \text{Im } \chi_{\text{opt}} \geq 0. \quad (20.100d)$$

### 20.2.3. The Feshbach projection operator formalism

We shall now examine an alternative way of relating the optical potential to the many-body problem, which is due to Feshbach [10]. Originally devised to study nuclear collision processes, the Feshbach method has also been applied to atomic collisions. The Feshbach formalism is able to take into account the Pauli principle between the incident and target particles and provides a particularly elegant description of *resonance scattering*. Although the Feshbach method may be applied to a variety of collision processes, we shall concentrate our attention here on resonance scattering, assuming that the incident particle is not energetic enough to excite the target so that only elastic scattering is allowed. This study of low-energy resonance scattering therefore supplements our previous analysis of the optical model at high energies.

Let us begin by defining a *projection operator*  $P$  which, acting on the full scattering wave function  $\Psi_a$  [23] is such that

$$\begin{aligned} P\Psi_a &\rightarrow \Psi_a \\ r &\rightarrow \infty \\ r_1 &\rightarrow \infty \\ &\vdots \\ r_j &\rightarrow \infty \end{aligned} \quad . \quad (20.101)$$

where  $\mathbf{r}$  is the incident particle coordinate and  $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j$  are the coordinates of target particles which are identical to the incident one. For example, in the case of a nucleon incident on a nucleus which contains  $N$  nucleons and is described by the wave function  $\psi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ , we may write

$$P\Psi_a(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \mathcal{A}\varphi(\mathbf{r})\psi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \quad (20.102)$$

where  $\mathcal{A}$  is the antisymmetrization operator and we have only displayed the space coordinates of the particles. From eq. (20.102) we deduce that if  $\Psi_a$  is the antisymmetrized wave function of the system, the function  $\varphi(\mathbf{r})$  yields asymptotically both the direct and exchange scattering amplitudes. Let us now introduce a second operator  $Q$  defined by the relation

$$Q = 1 - P. \quad (20.103)$$

Since  $P$  is a projection operator, it is such that

$$P^2 = P. \quad (20.104a)$$

Hence  $Q$  is also a projection operator, since

$$Q^2 = (1 - P)^2 = I - 2P + P^2 = I - P = Q. \quad (20.104b)$$

From eqs. (20.103) and (20.104) we also deduce that the operators  $P$  and  $Q$  are orthogonal, so that

$$PQ = QP = 0. \quad (20.105)$$

The total wave function  $\Psi_a$  satisfies the Schrödinger equation

$$(H - E_a)\Psi_a = 0 \quad (20.106)$$

where  $H$  is the full Hamiltonian of the many-body system. Let us break the total wave function  $\Psi_a$  into two parts as

$$\Psi_a = P\Psi_a + Q\Psi_a. \quad (20.107)$$

We note that because of eqs. (20.101) and (20.103) the component  $Q\Psi_a$  vanishes asymptotically. Using eq. (20.107), we may write the Schrödinger equation (20.106) as

$$(H - E_a)(P + Q)\Psi_a = 0.$$

Acting on this equation with  $P$  and  $Q$ , and using eqs. (20.104) and (20.105), we get

$$(H_{PP} - E_a)P\Psi_a + H_{PQ}Q\Psi_a = 0 \quad (20.108a)$$

$$(H_{QQ} - E_a)Q\Psi_a + H_{QP}P\Psi_a = 0 \quad (20.108b)$$

where

$$H_{PP} = PHP, H_{QQ} = QHQ, H_{PQ} = PHQ, H_{QP} = QHP. \quad (20.109)$$

The two equations (20.108) may be formally decoupled by solving first eq. (20.108b) for  $Q\Psi_a$ ,

$$Q\Psi_a = (E_a - H_{QQ})^{-1}H_{QP}P\Psi_a \quad (20.110)$$

and inserting this result into eq. (20.108a), so that

$$\{H_{PP} - E_a + H_{PQ}(E_a - H_{QQ})^{-1}H_{QP}\}P\Psi_a = 0. \quad (20.111)$$

We note from eq. (20.101), that even though  $P\Psi_a$  may differ from  $\Psi_a$  over all finite regions of configuration space, the solution of eq. (20.111) for  $P\Psi_a$  will lead to the exact elastic scattering amplitude. We may therefore rewrite eq. (20.111) as

$$(\mathcal{H}_{\text{eff}} - E_a)P\Psi_a = 0 \quad (20.112)$$

where

$$\mathcal{H}_{\text{eff}} = H_{PP} + \mathcal{V} \quad (20.113)$$

is the effective Hamiltonian for elastic scattering (i.e. the “equivalent” Hamiltonian for the wave function  $P\Psi_a$ ) and

$$\mathcal{V} = H_{PQ}(E_a - H_{QQ})^{-1}H_{QP} \quad (20.114)$$

is a complicated, non-local operator, which, as we shall see, is closely related to the optical potential.

A simple illustration of the above formulae may be illuminating at this point. Let us consider a case for which the incident particle is distinct from the target scatterers (e.g. positron-atom scattering). We may then choose  $P$  as the operator projecting on the target ground state  $|0\rangle$ , namely

$$P = |0\rangle\langle 0|. \quad (20.115)$$

Writing the total Hamiltonian  $H$  as

$$H = K + h + V_d$$

where  $K$  is the relative kinetic energy,  $h$  is the target Hamiltonian such that

$$h|0\rangle = w_0|0\rangle$$

and  $V_d$  is the full interaction between the incident and target particles, we find that eq. (20.112) becomes

$$[K + \langle 0|V_d|0\rangle + \mathcal{V} - E]P\Psi_a = 0 \quad (20.116)$$

with

$$E = E_a - w_0.$$

Thus, introducing the optical potential

$$\mathcal{V}_{\text{opt}} = \langle 0|V_d|0\rangle + \mathcal{V}$$

or

$$\mathcal{V}_{\text{opt}} = \langle 0|V_d|0\rangle + H_{PQ}(E_a - H_{QQ})^{-1} H_{QP} \quad (20.117)$$

we may write eq. (20.116) as

$$[K + \mathcal{V}_{\text{opt}} - E]P\Psi_a = 0. \quad (20.118)$$

Let us now return to the general case, described by eq. (20.112), and analyze in more detail the operator  $\mathcal{V}$  given by eq. (20.114). Following Feshbach, we shall show that *resonances arise from the presence of zeros in the denominator of the operator  $\mathcal{V}$* . To see how this comes about, let us imagine that we have solved the eigenvalue problem

$$H_{QQ}\chi_v = \varepsilon_v\chi_v \quad (20.119)$$

for all  $\varepsilon_v, \chi_v$ . We note that while the operators  $H$  and  $H_{PP}$  have a continuous spectrum in the scattering region, it follows from eqs. (20.101) and (20.103) that the eigenvalues  $\varepsilon_v$  are discrete below the excitation threshold. We also see from eq. (20.119) that the wave functions  $\chi_v$  are bound state solutions of an equation obtained from eq. (20.108b) by omitting the term  $H_{QP}P\Psi_a$  which permits the decay of  $Q\Psi_a$  into  $P\Psi_a$ . Now a resonance state of the compound system (incident particle plus target) has a very long lifetime with respect to typical collision times, and its probability of re-entering an open channel (here the elastic channel) is small. We may therefore, in first approximation, interpret the wave function  $\chi_v$  (corresponding to a state of infinite lifetime) as a *resonance state*, while the resonance energy is given approximately by  $\varepsilon_v$ . Such resonances are often called *Feshbach resonances*. It is worth noting that other resonances, called *shape resonances* may also arise when the potential in the single channel Schrödinger equation (20.118) has the right shape and strength to induce a resonant state. Since we have discussed such shape resonances at length in Chapter 4 we shall consider here only the Feshbach resonances. Using eqs. (20.119) and (20.104b), we have

$$H_{QQ}(Q\chi_v) = \varepsilon_v(Q\chi_v) \quad (20.120)$$



so that, assuming  $\varepsilon_v$  to be non-degenerate, we obtain

$$Q\chi_v = \lambda\chi_v.$$

Moreover, since  $Q^2 = Q$ , we have  $\lambda = 1$ , or

$$Q\chi_v = \chi_v \text{ (all } v). \quad (20.121)$$

Thus, from eqs. (20.119) and (20.121) we see that the  $\chi_v$  are simultaneous eigenstates of the operators  $H_{QQ}$  and  $Q$  with respective eigenvalues  $\varepsilon_v$  and 1. Furthermore, we deduce from eq. (20.121) that

$$PQ\chi_v = P\chi_v$$

or, using eq. (20.105),

$$P\chi_v = 0. \quad (20.122)$$

Finally, the completeness of the set  $\chi_v$  in the  $Q$  subspace allows us to write

$$Q = \sum_v |\chi_v\rangle\langle\chi_v|. \quad (20.123)$$

We are now prepared to examine the operator  $\mathcal{V}$  given by eq. (20.114). We first write

$$\mathcal{V} = H_{PQ}(E_a - H_{QQ})^{-1}QH_{QP}$$

where we have used the fact that  $QH_{QP} = Q^2HP = QHP = H_{QP}$ . Using eq. (20.123), we also have

$$\mathcal{V} = \sum_v H_{PQ}(E_a - H_{QQ})^{-1}|\chi_v\rangle\langle\chi_v|H_{QP}.$$

But, from eq. (20.119),

$$(E_a - H_{QQ})^{-1}|\chi_v\rangle = (E_a - \varepsilon_v)^{-1}|\chi_v\rangle \quad (20.124)$$

and therefore

$$\mathcal{V} = \sum_v H_{PQ} \frac{|\chi_v\rangle\langle\chi_v|}{E_a - \varepsilon_v} H_{QP} \quad (20.125)$$

so that eq. (20.112) becomes

$$\left[ H_{PP} + \sum_v H_{PQ} \frac{|\chi_v\rangle\langle\chi_v|}{E_a - \varepsilon_v} H_{QP} - E_a \right] P\Psi_a = 0. \quad (20.126)$$

If the resonances may be considered as isolated, so that the  $\varepsilon_v$  are well separated, it is clear from eq. (20.126) that when  $E_a$  gets very close to some  $\varepsilon_v$ , then one term in the sum on  $v$  will become very large. Let us isolate that particular term, say  $v = s$  by writing eq. (20.126) as

$$[H' - E_a]P\Psi_a = - H_{PQ} \frac{|\chi_s\rangle\langle\chi_s|}{E_a - \varepsilon_s} H_{QP} P\Psi_a \quad (20.127)$$

where

$$H' = H_{PP} + \sum_{v \neq s} H_{PQ} \frac{|\chi_v\rangle\langle\chi_v|}{E_a - \varepsilon_v} H_{QP} \quad (20.128)$$

is that part of the effective Hamiltonian which varies slowly with energy and therefore gives rise to the non-resonant part of the scattering.

To solve eq. (20.127), we first consider the solution  $P\hat{\Psi}_a$  of the corresponding homogeneous equation, namely

$$(H' - E_a)P\hat{\Psi}_a = 0 \quad (20.129)$$

which describes non-resonant scattering. Let us assume that we have been able to find outgoing spherical wave solutions of eq. (20.129), which we denote by  $P\hat{\Psi}_a^{(+)}$ . Then, defining the Green's operator

$$G_P^{(+)}(E_a) = \frac{1}{E_a - H' + i\varepsilon} = \left\{ E_a - H_{PP} - \sum_{v \neq s} H_{PQ} \frac{|\chi_v\rangle\langle\chi_v|}{E_a - \varepsilon_v} H_{QP} + i\varepsilon \right\}^{-1} \quad (20.130)$$

we find that the full wave function  $P\Psi_a^{(+)}$  which exhibits an outgoing spherical wave behaviour satisfies the equation

$$|P\Psi_a^{(+)}\rangle = |P\hat{\Psi}_a^{(+)}\rangle + G_P^{(+)} \frac{H_{PQ}|\chi_s\rangle\langle\chi_s|H_{QP}|P\Psi_a^{(+)}\rangle}{E_a - \varepsilon_s}. \quad (20.131)$$

The matrix element  $\langle\chi_s|H_{QP}|P\Psi_a^{(+)}\rangle$  may be obtained as follows. We have

$$\langle\chi_s|H_{QP}|P\Psi_a^{(+)}\rangle = \langle\chi_s|H_{QP}|P\hat{\Psi}_a^{(+)}\rangle + \frac{\langle\chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle}{E_a - \varepsilon_s} \langle\chi_s|H_{QP}|P\Psi_a^{(+)}\rangle$$

so that

$$\langle\chi_s|H_{QP}|P\Psi_a^{(+)}\rangle = \frac{\langle\chi_s|H_{QP}|P\hat{\Psi}_a^{(+)}\rangle}{1 - \langle\chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle/(E_a - \varepsilon_s)}. \quad (20.132)$$

Substituting this expression into eq. (20.131), we obtain

$$|P\Psi_a^{(+)}\rangle = |P\hat{\Psi}_a^{(+)}\rangle + G_P^{(+)} \frac{H_{PQ}|\chi_s\rangle\langle\chi_s|H_{QP}|P\hat{\Psi}_a^{(+)}\rangle}{E_a - \varepsilon_s - \langle\chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle} \quad (20.133)$$

or

$$P\Psi_a^{(+)} = P\hat{\Psi}_a^{(+)} + A_s \frac{1}{E_a - H' + i\varepsilon} H_{PQ}\chi_s \quad (20.134)$$

with

$$A_s = \frac{\langle\chi_s|H_{QP}|P\hat{\Psi}_a^{(+)}\rangle}{E_a - \varepsilon_s - \langle\chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle}. \quad (20.135)$$

The transition matrix element  $\langle b|\mathcal{T}|a\rangle$  leading to a final state  $\Phi_b$  may be readily obtained by applying to eq. (20.134) the two-potential formulae of Section 17.3. Defining  $P\hat{\Psi}_b^{(-)}$  as a solution of eq. (20.129) which exhibits an incoming spherical wave behaviour, we have

$$\langle b|\mathcal{T}|a\rangle = \langle b|\mathcal{T}|a\rangle_{\text{N.R.}} + \langle b|\mathcal{T}|a\rangle_{\text{R}} \quad (20.136)$$

where  $\langle b|\mathcal{T}|a\rangle_{\text{N.R.}}$  is the transition matrix element arising from the asymptotic behaviour of  $P\hat{\Psi}_a^{(+)}$  and giving the *non-resonant* part of the scattering and

$$\begin{aligned}\langle b|\mathcal{T}|a\rangle_{\text{R}} &= A_s \langle P\hat{\Psi}_b^{(-)}|H_{PQ}|\chi_s\rangle \\ &= \frac{\langle P\hat{\Psi}_b^{(-)}|H_{PQ}|\chi_s\rangle \langle \chi_s|H_{QP}|P\hat{\Psi}_a^{(+)}\rangle}{E_a - \varepsilon_s - \langle \chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle}.\end{aligned}\quad (20.137)$$

This last expression clearly exhibits a resonance behaviour. If we write

$$A_s = \text{Re}\langle \chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle \quad (20.138)$$

and

$$\frac{1}{2}\Gamma_s = -\text{Im}\langle \chi_s|H_{QP}G_P^{(+)}H_{PQ}|\chi_s\rangle \quad (20.139)$$

then the “resonant” part  $\langle b|\mathcal{T}|a\rangle_{\text{R}}$  of the transition matrix element becomes

$$\langle b|\mathcal{T}|a\rangle_{\text{R}} = \frac{\langle P\hat{\Psi}_b^{(-)}|H_{PQ}|\chi_s\rangle \langle \chi_s|H_{QP}|P\hat{\Psi}_a^{(+)}\rangle}{E_a - (\varepsilon_s + A_s) + \frac{1}{2}i\Gamma_s}.\quad (20.140)$$

We see that the term  $A_s$  gives rise to a shift in the position of the resonance from  $\varepsilon_s$ , while the quantity  $\Gamma_s$  controls the width of the resonance: if  $\Gamma_s$  is small, then the resonance is narrow. We also note that if  $\chi_s$  is a state of definite angular momentum the resonance will occur in a given partial wave.

We may now briefly summarize the Feshbach method. By applying the projection operators  $P$  and  $Q$  one divides the total wave function into an open channel part  $P\Psi_a$  and a closed channel fraction  $Q\Psi_a$ . A Schrödinger equation for the open channel part is then obtained [eq. (20.112)] which involves an effective Hamiltonian. The analysis of the structure of this effective Hamiltonian may be reduced to the solution of the eigenvalue problem (20.119). The transition matrix element is then given by eqs. (20.136)–(20.140). We see that important steps in the Feshbach method are the construction of the appropriate projection operators and the solution of the eigenvalue equation (20.119). We shall return to these questions in Section 20.4.2 where we shall apply the Feshbach method to the study of low-energy electron–atomic hydrogen resonance scattering.

Before leaving the subject of formal resonance theory we list in reference [24] a few important papers dealing with the theory of resonant scattering.

### 20.3. High-energy elastic hadron–nucleus scattering

Consider a hadron  $X$  of initial laboratory energy  $E_L$  and wave vector  $k_L$  incident on a nucleus of mass number  $A$ . Assuming that the high-energy small angle conditions are satisfied, we may use the Glauber eikonal version of the optical model developed in Section 20.2.2 to write the elastic scattering amplitude in the laboratory system as

$$f_{\text{el}}^G = \frac{k_L}{2\pi i} \int d^2b \exp(i \mathbf{q} \cdot \mathbf{b}) [\exp\{i\chi_{\text{opt}}(\mathbf{b})\} - 1] \quad (20.141)$$

where  $\mathbf{q} = \mathbf{k}_L - \mathbf{k}'_L$  is the wave vector transfer in the laboratory system. The optical phase shift function  $\chi_{\text{opt}}$  appearing in eq. (20.141) is such that

$$\exp \{i\chi_{\text{opt}}(\mathbf{b})\} = \langle 0 | \exp \{i\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_A)\} | 0 \rangle \quad (20.142)$$

where

$$\chi_{\text{tot}}^G(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_A) = \sum_{j=1}^A \chi_j(\mathbf{b} - \mathbf{b}_j) \quad (20.143)$$

is the sum of the phase shifts contributed by each of the target nucleons. Here we have written the coordinate of the incoming hadron as

$$\mathbf{r} = \mathbf{b} + z\hat{\mathbf{z}}$$

while

$$\mathbf{r}_j = \mathbf{b}_j + z_j\hat{\mathbf{z}}$$

are the coordinates of the target nucleons and the  $z$ -axis is chosen along the bisector of the scattering angle. We assume that the individual phase shift functions  $\chi_j$  describing the scattering of the incident particle by the individual target nucleons are known and we neglect for the moment their possible spin or isospin dependence. We may also introduce the functions

$$\Gamma_j(\mathbf{b}) = 1 - \exp \{i\chi_j(\mathbf{b})\} \quad (20.144)$$

which vanish for  $\mathbf{b}$  outside the nuclear force range. From eq. (19.102), we note that

$$f_j = \frac{ik_L}{2\pi} \int d^2\mathbf{b} \exp(i\mathbf{q} \cdot \mathbf{b}) \Gamma_j(\mathbf{b}) \quad (20.145)$$

is precisely the eikonal two-body scattering amplitude of the incident particle by the  $j$ th nucleon (in the laboratory system). Then, using the fact that

$$\exp(i\chi_{\text{tot}}^G) = \exp \left\{ i \sum_{j=1}^A \chi_j(\mathbf{b} - \mathbf{b}_j) \right\} = \prod_{j=1}^A [1 - \Gamma_j(\mathbf{b} - \mathbf{b}_j)] \quad (20.146)$$

we may write the elastic scattering amplitude as

$$f_{\text{el}}^G = \frac{ik_L}{2\pi} \int d^2\mathbf{b} \exp(i\mathbf{q} \cdot \mathbf{b}) \langle 0 | \Gamma_{\text{tot}}(\mathbf{b}, \mathbf{b}_1, \dots, \mathbf{b}_A) | 0 \rangle \quad (20.147)$$

where  $\Gamma_{\text{tot}}$  is given by eq. (19.112), namely

$$\Gamma_{\text{tot}} = 1 - \prod_{j=1}^A [1 - \Gamma_j(\mathbf{b} - \mathbf{b}_j)] \quad (20.148)$$

and may be written in the form of a multiple scattering expansion, namely

$$\Gamma_{\text{tot}} = \sum_{j=1}^A \Gamma_j - \sum_{j \neq l} \Gamma_j \Gamma_l + \dots + (-1)^{A-1} \prod_{j=1}^A \Gamma_j. \quad (20.149)$$

Let us analyze more closely the contribution to  $f_{\text{el}}^G$  arising from the first term (or "single scattering" term) on the right-hand side of eq. (20.149). Using eq. (20.145) we immediately deduce that this "single scattering" or *impulse approximation* (I.A.) leads to the elastic scattering amplitude

$$f_{\text{el}}^{\text{IA}} = \sum_{j=1}^A f_j \langle 0 | \exp(i\mathbf{q} \cdot \mathbf{b}_j) | 0 \rangle. \quad (20.150)$$

Furthermore, if we assume that all the  $f_j$  are identical ( $f_1 = f_2 = \dots = f$ ), and use the fact that they only depend on the (laboratory) wave vector transfer  $\mathbf{q} = (\mathbf{k}_1 - \mathbf{k}'_1)$ , we may write the differential cross section for elastic scattering in the impulse approximation as

$$\frac{d\sigma_{el}^A}{d\Omega} = A^2 (d\sigma/d\Omega)_f |S(\mathbf{q})|^2 \quad (20.151)$$

where

$$(d\sigma/d\Omega)_f = |f|^2$$

is the elastic differential cross section for the scattering of the incident particle by a *free* nucleon, and

$$S(\mathbf{q}) = A^{-1} \sum_{j=1}^A \langle 0 | \exp(i\mathbf{q} \cdot \mathbf{r}_j) | 0 \rangle \quad (20.152)$$

is the elastic *form factor* [25] of the target bound state. Since  $S(0) = 1$ , the formula (20.151) predicts that in the impulse approximation the coherent (elastic) differential cross section for hadron-nucleus scattering is enhanced by a factor  $A^2$  in the forward direction with respect to the hadron-nucleon cross section. In practice, since hadrons and nucleons interact strongly, multiple scattering effects are important in nuclei. They lead to an  $A$ -dependence of the forward differential cross section which increases less rapidly than  $A^2$  although the general tendency of the angular distribution to be concentrated in the forward direction remains. This strong forward peaking is the main characteristic of high energy coherent hadron-nucleus scattering.

In order to improve on the impulse approximation we follow the treatment of Glauber [9] and return to the general formulae (20.141) and (20.147) for the elastic scattering amplitude. We then have, from eqs. (20.142) and (20.146)

$$\exp\{i\chi_{opt}(\mathbf{b})\} = \left\langle 0 \left| \prod_{j=1}^A [1 - \Gamma_j(\mathbf{b} - \mathbf{b}_j)] \right| 0 \right\rangle. \quad (20.153)$$

It is convenient at this point to use an independent particle model for the nucleus. Then the nuclear ground state wave function factorizes and we have (neglecting exchange effects in the target)

$$|\psi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)|^2 = \prod_{j=1}^A \rho_j(\mathbf{r}_j) \quad (20.154)$$

where  $\rho_j(\mathbf{r}_j)$  is the density for the  $j$ th particle, normalized to unity. We may then write eq. (20.153) as

$$\exp\{i\chi_{opt}(\mathbf{b})\} = \prod_{j=1}^A \left\{ 1 - \int \rho_j(\mathbf{r}_j) \Gamma_j(\mathbf{b} - \mathbf{b}_j) d\mathbf{r}_j \right\} \quad (20.155)$$

from which we deduce that

$$\chi_{opt}(\mathbf{b}) = -i \sum_{j=1}^A \log \left\{ 1 - \int \rho_j(\mathbf{r}_j) \Gamma_j(\mathbf{b} - \mathbf{b}_j) d\mathbf{r}_j \right\}. \quad (20.156)$$

Let us now consider the expression

$$B_j(\mathbf{b}) = \int \rho_j(\mathbf{r}_j) \Gamma_j(\mathbf{b} - \mathbf{b}_j) d\mathbf{r}_j. \quad (20.157)$$

This quantity vanishes when  $\mathbf{b}$  is appreciably larger than the nuclear radius, and its order of magnitude when  $\mathbf{b}$  is inside the nucleus is easily obtained. Indeed, we know that

$$\Gamma_j(\mathbf{b} - \mathbf{b}_j) = 1 - \exp[i\chi_j(\mathbf{b} - \mathbf{b}_j)]$$

is zero outside of a small pencil, centered about a line  $\mathbf{b} = \text{constant}$ , and of radius  $a$ , where  $a$  is the interaction range between the incident particle and a target nucleon. In the interior of this pencil, the quantity  $\Gamma_j$  is at most of order unity. Since  $\rho_j$  is inversely proportional to  $R^3$  – where  $R$  is the radius of the nucleus – while the volume of the pencil is proportional to  $a^2 R$ , we deduce that  $B_j(\mathbf{b})$  is of order  $a^2/R^2$  and is therefore quite small compared to unity, even in the case of a nucleus of moderate size. We may therefore expand the arguments of the logarithms in eq. (20.156) and write

$$\chi_{\text{opt}}(\mathbf{b}) \simeq i \sum_{j=1}^A \int \rho_j(\mathbf{r}_j) \Gamma_j(\mathbf{b} - \mathbf{b}_j) d\mathbf{r}_j. \quad (20.158)$$

Since we are presently neglecting all isospin effects, all the functions  $\Gamma_j$  are the same and we may also introduce the average particle density

$$\rho = \frac{1}{A} \sum_{j=1}^A \rho_j \quad (20.159)$$

to write the optical phase shift as

$$\chi_{\text{opt}}(\mathbf{b}) = iA \int \rho(\mathbf{r}') \Gamma(\mathbf{b} - \mathbf{b}') d\mathbf{r}' \quad (20.160)$$

where we have used the variable  $\mathbf{r}' = \mathbf{b}' + z'\hat{\mathbf{z}}$  instead of  $\mathbf{r}_j$ .

At the expense of a further approximation, we may still simplify eq. (20.160) as follows. Writing

$$\rho(\mathbf{r}') = \rho(\mathbf{b}', z')$$

and changing variables to  $\mathbf{b}'' = \mathbf{b} - \mathbf{b}'$ , we have

$$\chi_{\text{opt}}(\mathbf{b}) = iA \int \rho(\mathbf{b} - \mathbf{b}'', z') \Gamma(\mathbf{b}'') d^2\mathbf{b}'' dz'. \quad (20.161)$$

Now the nuclear density is practically constant over a large fraction of the nucleus, while  $\Gamma$  is non-vanishing only over a small region of the  $\mathbf{b}''$  plane. We may therefore expand the nuclear density in a Taylor series about  $\mathbf{b}$ , and neglect terms of order  $a^2/R^2$  to obtain (with  $z' \rightarrow z$ )

$$\chi_{\text{opt}}(\mathbf{b}) = iA \int_{-\infty}^{+\infty} \rho(\mathbf{b}, z) dz \int d^2\mathbf{b}'' \Gamma(\mathbf{b}''). \quad (20.162)$$

But from eq. (20.145) we see that the quantity

$$f_L(0) = \frac{ik_L}{2\pi} \int d^2\mathbf{b} \Gamma(\mathbf{b}) \quad (20.163)$$

is precisely the forward scattering amplitude for hadron-nucleon elastic scattering (in the lab. system). Thus we may write

$$\chi_{\text{opt}}(\mathbf{b}) = \frac{2\pi A}{k_L} f_L(0) \int_{-\infty}^{+\infty} \rho(\mathbf{b}, z) dz \quad (20.164)$$

which is a very simple expression for the optical phase shift function. We see that it involves only the de Broglie wavelength  $\lambda = 2\pi/k_L$  of the incident particle, the density and mass number of the target nucleus, and the hadron-nucleon elastic scattering amplitude in the forward direction. Using eq. (20.96) we may also deduce from (20.164) the corresponding optical potential

$$V_{\text{opt}}(\mathbf{r}) = -\frac{2\pi\hbar v_i}{k_L} A f_L(0) \rho(\mathbf{r}) \quad (20.165)$$

where  $v_i$  is the relative initial velocity. Since

$$v_i = \hbar c^2 k_L / E_L$$

we have

$$V_{\text{opt}}(\mathbf{r}) = -\frac{2\pi\hbar^2 c^2}{E_L} A f_L(0) \rho(\mathbf{r}). \quad (20.166)$$

We may also use the optical theorem to write

$$V_{\text{opt}}(\mathbf{r}) = -\frac{2\pi\hbar^2 c^2}{E_L} A \rho(\mathbf{r}) \left[ \text{Re } f_L(0) + i \frac{k_L}{4\pi} \sigma_{\text{XN}} \right] \quad (20.167)$$

where  $\sigma_{\text{XN}}$  is the total hadron-nucleon cross section. Finally, we note that the complex refractive index introduced in Section 20.1.2 is given by

$$n(\mathbf{r}) = 1 + \frac{2\pi A}{k_L^2} f_L(0) \rho(\mathbf{r}). \quad (20.168)$$

Let us briefly review the approximations which lead to our final results (20.164) and (20.166). Apart from the conditions of validity of the eikonal approximation (high incident wave number and small angle scattering), we have also used an independent particle model for the nucleus and neglected terms of order  $a^2/R^2$ .

It is instructive to compare the expressions which we have just obtained for  $\chi_{\text{opt}}$  with those following from the impulse approximation  $\Gamma_{\text{tot}} \simeq \Sigma_j \Gamma_j$ . In the latter case one has

$$\exp\{i\chi_{\text{opt}}(\mathbf{b})\} \simeq \langle 0 | 1 - \sum_{j=1}^A \Gamma_j(\mathbf{b} - \mathbf{b}_j) | 0 \rangle. \quad (20.169)$$

Using again an independent particle nuclear model, we have then

$$\chi_{\text{opt}}(\mathbf{b}) \simeq -i \log \left\{ 1 - \sum_{j=1}^A \int \rho_j(\mathbf{r}_j) \Gamma(\mathbf{b} - \mathbf{b}_j) d\mathbf{r}_j \right\} \quad (20.170)$$

and the approximations which we used to obtain eq. (20.164) now give [26]

$$\chi_{\text{opt}}(\mathbf{b}) \simeq -i \log \left\{ 1 + A \frac{2\pi i}{k_L} f_L(0) \int_{-\infty}^{+\infty} \rho(\mathbf{b}, z) dz \right\}. \quad (20.171)$$

We note the presence of the summation inside the argument of the logarithm in eq. (20.170) – or the factor  $A$  inside this argument in eq. (20.171) – so that we may only obtain the results (20.158) and (20.164) from eqs. (20.170) and (20.171) when  $A$  is relatively small. This is in accordance with the fact that multiple scattering terms in eq. (20.149), responsible for absorption, shadow, interference effects, etc., are more likely to influence the small angle elastic scattering in a large nucleus than in a small one.

Let us now return to the basic formulae (20.164) and (20.166) which we have obtained for  $\chi_{\text{opt}}$  and  $V_{\text{opt}}$ . We first recall that these expressions have been established in the *laboratory system*. It is a simple matter, however, to obtain formulae which involve the C.M. quantities  $k$  and  $f(0)$ . Since the ratio of the forward amplitude divided by the momentum is a relativistic invariant, we may write

$$\chi_{\text{opt}}(\mathbf{b}) = \frac{2\pi A}{k} f(0) \int_{-\infty}^{+\infty} \rho(\mathbf{b}, z) dz \quad (20.172)$$

and

$$V_{\text{opt}}(\mathbf{r}) = - \frac{2\pi\hbar^2 c^2}{E_L} \frac{k_L}{k} A f(0) \rho(\mathbf{r}). \quad (20.173)$$

It is important to note that the equations (20.166) or (20.173) for the optical potential, which we have derived within the framework of the Glauber eikonal theory, may also be obtained from an analysis of the first term of the Watson multiple scattering series (20.87) for the optical potential [27]. Hence the “single scattering” approximation of Watson (keeping only the first term on the right-hand side of eq. (20.87) for the optical potential) should not be confused with the single scattering (impulse) approximation of Glauber, which amounts to keeping only the first term on the right-hand side of eq. (20.149) and leads to the impulse approximation results (20.151), (20.170) and (20.171).

Let us now discuss some corrections to the formulae (20.164) and (20.166)

(i) *Spin effects*. To order  $A^{-1}$ , where  $A$  is the mass number, there are as many nucleons with spin up as with spin down at any point of a nucleus in its ground state [28]. Therefore the quantities  $f_L(0)$  or  $f(0)$  which appear in the above formulae must be averaged over the target nucleon spin. This spin averaging makes the nuclear scattering sensitive to a different amplitude from that which describes forward scattering on a free target nucleon. Hence, the comparison of results with nucleons and nuclei as targets may permit the isolation of spin-dependent effects.

As an illustration of the role of spin effects in high-energy hadron–nucleus scattering, let us assume that the scattering of the incident particle by a target nucleon contains a spin-orbit term. Then the laboratory two-body hadron–nucleon scattering amplitude may be written in the form (see Section 18.3)

$$M = f(\mathbf{k}'_L, \mathbf{k}_L) + \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} g(\mathbf{k}'_L, \mathbf{k}_L) \quad (20.174)$$



where  $f$  and  $g$  are spin independent amplitudes,  $\sigma$  is the Pauli spin matrix and

$$\hat{n} = \frac{\mathbf{k}_L \times \mathbf{k}'_L}{|\mathbf{k}_L \times \mathbf{k}'_L|}$$

is a unit vector perpendicular to the plane of scattering. Furthermore, the scattering amplitude  $g$  vanishes in the forward direction, so that no spin-orbit term is obtained in the approximation which led us to eq. (20.166). However, if we return to eq. (20.161) and keep the next term in the expansion of the average density it may be shown [9] that

$$V_{\text{opt}}(r) = -\frac{2\pi\hbar^2 c^2}{E_L} A \left[ f_L(0)\rho(r) + \frac{i}{k_L} g'_L(0) \frac{1}{r} \frac{d}{dr} \rho(r) \sigma \cdot L \right] \quad (20.175)$$

where the average density is assumed to be spherically symmetric and

$$g'_L(0) = |dg_L(\theta)/d\theta|_{\theta=0}.$$

For nuclei of small mass number  $A$  which cannot be considered as saturated spin systems and for which the concept of an average density has little meaning, the spin effects must be studied by other methods. An important case is hadron-deuteron scattering, for which spin effects have been investigated by several authors [29, 30] and found to be small at high energies.

(ii) *Isospin effects.* As in the case of spin effects, the amplitudes  $f_L(0)$  or  $f(0)$  must be averaged over the target nucleon isospin (to order  $A^{-1}$ ). We may thus rewrite eqs. (20.164) and (20.166) as

$$\chi_{\text{opt}}(\mathbf{b}) = \frac{2\pi A}{k_L} \bar{f}_L(0) \int_{-\infty}^{+\infty} \rho(\mathbf{b}, z) dz \quad (20.176)$$

and

$$V_{\text{opt}}(\mathbf{r}) = -\frac{2\pi\hbar^2 c^2}{E_L} A \bar{f}_L(0) \rho(\mathbf{r}) \quad (20.177)$$

where

$$\bar{f}_L(0) = \frac{1}{A} [Z f_{xp}(0) + N f_{xn}(0)] \quad (20.178)$$

is the mean forward scattering amplitude,  $Z$  being the number of protons and  $N$  the number of neutrons in the target nucleus, while  $f_{xp}(0)$  and  $f_{xn}(0)$  are respectively the forward scattering amplitudes for hadron-proton and hadron-neutron scattering.

(iii) *Correlation effects.* We have described so far the nucleus by an independent particle model. In fact, various types of correlations in the position or spin variables may arise between the target nucleons. For example, attractive or repulsive interactions between the nucleons may lead to deviations from the independent particle model. Even in the absence of such

interactions, the *Pauli exclusion principle* already introduces a correlation between the nucleons, since two similar fermions are not allowed to have the same spatial and spin coordinates. In general these correlation effects are complicated to analyze. We refer the reader to the references [8, 9, 11, 31] for a discussion of this subject.

(iv) *Coulomb effects*. If the incident hadron is a charged particle, it is of course necessary to take into account the long-range Coulomb forces [32] as well as the short-range strong forces. This is a typical “two-potential” problem which is particularly easy to solve in the eikonal approximation where the relations between the phase shift functions and the interaction potentials are linear. There is however an additional subtlety, since the

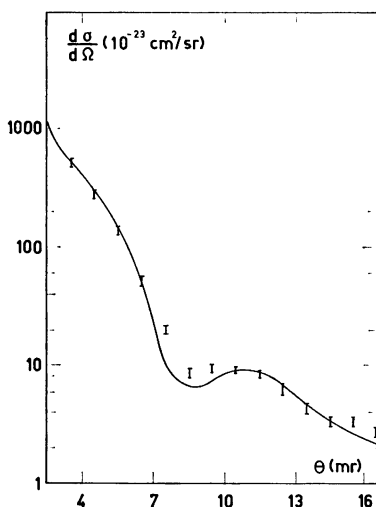


Fig. 20.3. Laboratory differential cross section for proton scattering on copper at 19.3 GeV/c, in units of  $10^{-23} \text{ cm}^2/\text{sr}$ . The experimental points are from Belletini *et al.* [34]. The theoretical curve uses a Woods-Saxon nuclear density with  $R = 4.3 \text{ fm}$ ,  $a = 0.55 \text{ fm}$  (taken from Goldhaber and Joachain [31]).

actual Coulomb potential inside the nucleus is that of an extended charge distribution [33]. For high energy scattering of protons from nuclei of large  $Z$  (such as lead) the Coulomb amplitude turns out to be comparable to the nuclear amplitude, so that a precise calculation of Coulomb effects is important.

As an example of high-energy hadron-nucleus elastic scattering, we show in Figs. 20.3 and 20.4 the angular distributions corresponding to proton scattering on copper and lead nuclei at 19.3 GeV/c incident laboratory momentum. The theoretical curves have been obtained by using eq. (20.164), corrected for spin, isospin, correlation and Coulomb effects [31]. The experimental points are those of Belletini *et al.* [34].

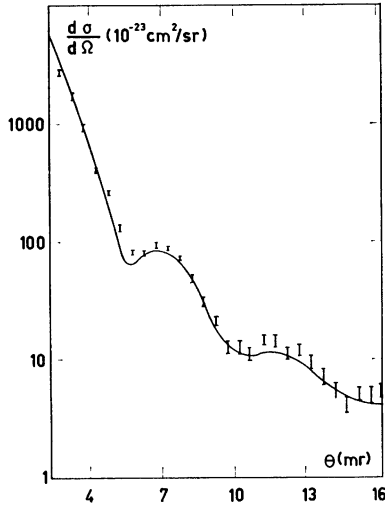


Fig. 20.4. Laboratory differential cross section for proton scattering on lead at 19.3 GeV/c, in units of  $10^{-23} \text{ cm}^2/\text{sr}$ . The experimental points are those of Belletini *et al.* [34]. The theoretical curve uses a Woods-Saxon nuclear density with  $R = 6.5 \text{ fm}$ ,  $a = 0.7 \text{ fm}$  (taken from Goldhaber and Joachain [31]).

## 20.4. Elastic scattering of charged particles by atoms

Let us consider the elastic scattering of a particle A of mass  $m_A$  and charge  $Qe$  by a neutral atom B having  $Z$  electrons. We suppose that the collision is non-relativistic, and assume that the center of mass of the atom coincides with its nucleus. We shall treat the collision in the C.M. system, using the relative coordinates  $\mathbf{r}$  which joins the position of the nucleus to that of the particle A and  $\mathbf{r}_j$  ( $j = 1, 2, \dots, Z$ ) which determine the positions of the atomic electrons with respect to the nucleus (see Fig. 20.5). The center of mass wave vectors in the initial and final state are  $\mathbf{k}_i$  and  $\mathbf{k}_f$ , with  $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ .

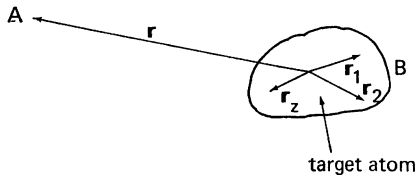


Fig. 20.5. Illustration of the coordinates  $\mathbf{r}$  and  $\mathbf{r}_j$  of the text.

The complete Hamiltonian of the system (A + B) may be written as

$$H = H_a + V_a \quad (20.179)$$

where  $H_d$ , the “unperturbed” Hamiltonian describing the free motion of the two particles A and B in the elastic channel (i.e. the motion of A and B when they are far apart) is given by the sum of the relative kinetic energy  $K$  and of the internal target Hamiltonian  $h$ . Therefore

$$H_d = K + h \quad (20.180)$$

where the operator  $K$  is given in the position representation by

$$K = -\frac{1}{2M}\nabla_r^2 \quad (20.181)$$

and

$$h = \sum_{i=1}^Z K_i + U \quad (20.182)$$

with

$$K_i = -\frac{1}{2}\nabla_{r_i}^2 \quad (20.183)$$

and

$$U = \sum_{i=1}^Z \left( -\frac{Z}{r_i} \right) + \sum_{i>j=1}^Z \frac{1}{r_{ij}}. \quad (20.184)$$

In the above formulae and in the remaining part of this section we use atomic units (a.u.), defined in footnote [45] of Chapter 19. We have also set  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$  and introduced the reduced mass

$$M = m_A m_B / (m_A + m_B) \quad (20.185)$$

where  $m_B$  is the mass of the target atom B. Furthermore, we have

$$h|n\rangle = w_n|n\rangle \quad (20.186)$$

and we shall assume that the atom is initially in the ground state  $|0\rangle$ , with an internal energy  $w_0$ .

The interaction  $V_d$  is the sum of the individual interactions of the incident particle A with the  $(Z + 1)$  particles of the target. We shall neglect all but the Coulomb interactions and write (in a.u.)

$$V_d = \frac{ZQ}{r} + \sum_{j=1}^Z v_j \quad (20.187)$$

with

$$v_j = -\frac{Q}{|\mathbf{r} - \mathbf{r}_j|}. \quad (20.188)$$

#### 20.4.1. The multiple scattering approach

Following Mittleman and Watson [35–38], let us first analyze this elastic scattering problem by determining the optical potential approximately from eq. (20.77). We shall neglect for the moment the possible effects of the Pauli principle between the incident particle and the target particles. Thus, if the

particle A is an electron we presently ignore exchange effects. As we have already noted above, the first term on the right-hand side of eq. (20.77) is simply the *static* potential  $V_{st} = \langle 0|V_d|0\rangle$ . Our first approximation to the optical potential may therefore be written as

$$V^{(1)}(\mathbf{r}) = V_{st}(\mathbf{r}) = \frac{ZQ}{r} - Q \sum_{j=1}^Z \left\langle 0 \left| \frac{1}{|\mathbf{r} - \mathbf{r}_j|} \right| 0 \right\rangle. \quad (20.189)$$

This expression may be readily evaluated for simple atoms [39] or when an independent particle model (such as the Hartree–Fock method) is used to describe the state  $|0\rangle$  of the target. The static potential (20.189) has been used frequently to describe the elastic scattering of charged particles by atoms. We already pointed out in our discussion of electron–atomic hydrogen elastic scattering (see Section 19.5) that the static interaction does not take into account several important features of the collision. For example, *polarization effects* (which we shall analyze below) are missing from  $V_{st}$ . Moreover, at C.M. energies above the excitation threshold of the target the static interaction (20.189), which is *real* does not take into account *absorption effects* due to the possibility of the removal of incident particles from the initial (elastic) channel [40]. Furthermore, if the incident particle is identical to one of the target scatterers, *exchange effects* must be taken into account. Such effects are obviously not present in  $V_{st}$ .

However, as we already remarked in Section 19.5, the static interaction (20.189) correctly reduces for small values of the relative distance  $r$  to the Coulomb interaction  $ZQ/r$  acting between the incident particle and the nucleus of the target atom. We therefore expect that the potential  $V_{st}$  will account for elastic (direct) collisions involving small relative distances. Therefore, if exchange effects between the incident particle and the target scatterers are not present or may be neglected, and when semi-classical conditions apply (i.e. when  $k \gg 1$ ), the static interaction (20.189) will describe correctly the *large angle* elastic scattering, which corresponds to small impact parameters. That this is the case for the elastic scattering of fast electrons by atomic hydrogen has already been shown in Section 19.5. We shall also illustrate this point in Section 21.1 while discussing elastic electron–helium scattering.

Let us now consider the second term on the right-hand side of eq. (20.77), namely

$$V^{(2)} = \sum_{n \neq 0} \frac{\langle 0|V_d|n\rangle \langle n|V_d|0\rangle}{k^2/2M - K - (w_n - w_0) + i\varepsilon} \quad (20.190)$$

where the summation runs over all the intermediate states of the target. Here  $k^2/2M$  is the relative kinetic energy,  $K$  is the kinetic energy operator (20.181),  $w_0$  and  $w_n$  represent the internal target energies respectively in the initial state  $|0\rangle$  and in the intermediate state  $|n\rangle$ , and  $\varepsilon \rightarrow 0^+$ .

The expression (20.190) is in general very difficult to evaluate, so that approximation methods must be used. We shall examine here two of these approximations.

(i) If we assume that the change  $(k^2/2M - K)$  in kinetic energy in the propagator  $[k^2/2M - K - (w_n - w_0) + i\varepsilon]^{-1}$  may be neglected, we may rewrite eq. (20.190) as

$$V_{\text{ad}}^{(2)} = \sum_{n \neq 0} \frac{\langle 0|V_d|n\rangle\langle n|V_d|0\rangle}{w_0 - w_n} \quad (20.191)$$

where we have now omitted the prescription  $\varepsilon \rightarrow 0^+$  since the denominator appearing in eq. (20.191) is no more singular. The approximation leading to eq. (20.191) is called the *adiabatic approximation*. We note that since the interaction  $V_d$  is local, the adiabatic expression (20.191) yields a *local* second order potential  $V_{\text{ad}}^{(2)}(\mathbf{r})$ , and therefore a *local* optical potential

$$V_{\text{opt}}(\mathbf{r}) = V^{(1)}(\mathbf{r}) + V_{\text{ad}}^{(2)}(\mathbf{r}) \quad (20.192)$$

since  $V^{(1)}(\mathbf{r})$  is evidently local. Furthermore, because  $V_{\text{ad}}^{(2)}(\mathbf{r})$  is obviously *real*, the optical potential  $V_{\text{opt}}(\mathbf{r})$  computed from eq. (20.192) suffers from the same defect as  $V^{(1)}(\mathbf{r})$  at energies lying above the first excitation threshold (i.e. it does not account for the removal of particles from the elastic channel).

In order to obtain a simple expression for  $V^{(2)}$  in the adiabatic approximation, let us examine what happens when the coordinate  $r$  of the incoming particle is large compared to the size of the target atom. Returning to the expression (20.188) of the Coulomb interaction between the incident particle and an atomic electron, we first write

$$v_j = -Q \frac{1}{|\mathbf{r} - \mathbf{r}_j|} = -Q \sum_{l=0}^{\infty} \frac{(r_<)^l}{(r_>)^{l+1}} P_l \left( \frac{\mathbf{r} \cdot \mathbf{r}_j}{rr_j} \right)$$

where  $r_<$  is the lesser and  $r_>$  the greater of  $r$  and  $r_j$ . For  $r > r_j$  we therefore have

$$v_j \simeq -Q \left[ \frac{1}{r} + \frac{1}{r^2} \hat{\mathbf{r}} \cdot \mathbf{r}_j + \dots \right]$$

where  $\hat{\mathbf{r}}$  is the unit vector along  $\mathbf{r}$ . Thus, neglecting higher order terms in  $r^{-1}$ , we have

$$\sum_{j=1}^Z v_j \simeq -\frac{ZQ}{r} - \frac{Q}{r^2} \sum_{j=1}^Z \hat{\mathbf{r}} \cdot \mathbf{r}_j \quad (20.193)$$

and the interaction  $V_d$  given by eq. (20.187) becomes for large  $r$

$$V_d(r) \simeq -\frac{Q}{r^2} \sum_{j=1}^Z \hat{\mathbf{r}} \cdot \mathbf{r}_j. \quad (20.194)$$

The adiabatic approximation (20.191) to the second order optical potential then becomes

$$V_{\text{ad}}^{(2)}(\mathbf{r}) \simeq -\frac{\bar{\alpha}Q^2}{2i^4} \quad (20.195)$$

where

$$\bar{\alpha} = 2 \sum_{n \neq 0} \frac{|\langle 0 | \hat{p} \cdot \sum_{j=1}^Z \mathbf{r}_j | n \rangle|^2}{w_n - w_0} \quad (20.196)$$

is the *atomic dipole polarizability*, a quantity which is rather tractable to evaluate [41], or may also be obtained directly from experiment. Thus we see from eq. (20.195) that intermediate excited states of the target give rise to a *long range* potential which behaves like  $r^{-4}$  for large values of  $r$ .

The approximate expression (20.195) which we have obtained for  $V_{\text{ad}}^{(2)}$  is of course invalid for values of  $r$  which are not large with respect to typical atomic dimensions. For example at  $r = 0$  we see that the expression (20.195) exhibits an  $r^{-4}$  singularity. A simple, phenomenological way of trying to extend the validity of (20.195) down to  $r = 0$  is to introduce a "cut-off" parameter  $d$  so that  $V_{\text{ad}}^{(2)}$  becomes

$$V_{\text{ad}}^{(2)}(r) \simeq V_p(r) = - \frac{\bar{\alpha} Q^2}{2(r^2 + d^2)^2}. \quad (20.197)$$

This form is called the Buckingham polarization potential [42] and has been widely used in the description of elastic scattering of charged particles by atoms. The cut-off parameter  $d$  is a length related to the size of the atom. An estimate of  $d$ , based on the Thomas-Fermi model and the Schwinger variational principle yields [35]

$$d \simeq (\frac{1}{2} \bar{\alpha} Z^{-1/3})^{1/4}. \quad (20.198)$$

Mittleman and Watson [35–38] have investigated in detail the accuracy of the adiabatic approximation. They find that it is expected to improve with decreasing energies and large values of  $Z$ , and is always good at large distances from the atom. The error associated with the use of the Buckingham polarization potential is more difficult to evaluate, since the scattering at low energies is quite sensitive to the cut-off parameter  $d$ .

The extension of this method to include the effect of the Pauli principle when the incident particle is an electron has been given by Lippmann, Mittleman and Watson [43]. This analysis may be carried out in a simple way when Hartree-Fock wave functions are used to describe the internal state of the atom. In this case the optical model potential becomes the *non-local* operator

$$\langle \mathbf{r} | V_{\text{opt}} | \mathbf{r}' \rangle = \delta(\mathbf{r}' - \mathbf{r}) [V^{(1)}(\mathbf{r}) + V_p(r)] + \langle \mathbf{r} | V_{\text{ex}} | \mathbf{r}' \rangle + \langle \mathbf{r} | V_{\text{orth}} | \mathbf{r}' \rangle \quad (20.199)$$

where  $V^{(1)}(\mathbf{r})$  and  $V_p(r)$  are respectively the static and Buckingham polarization potentials defined above, while

$$\langle \mathbf{r} | V_{\text{ex}} | \mathbf{r}' \rangle = - \sum_{j=1}^Z \frac{1}{|\mathbf{r}' - \mathbf{r}|} \varphi_j(\mathbf{r}) \varphi_j^*(\mathbf{r}') \quad (20.200a)$$

and

$$\langle \mathbf{r} | V_{\text{orth}} | \mathbf{r}' \rangle = - \sum_{j=1}^Z \varphi_j(\mathbf{r}) \varphi_j^*(\mathbf{r}') V_p(\mathbf{r}'). \quad (20.200b)$$

Here the functions  $\varphi_j$  are the Hartree-Fock orbitals of the target atom. With the non-local potential (20.199), the Schrödinger equation for the scattering wave function  $\varphi_{k_{i,v,v_t}}^{(+)}$  then becomes an integro-differential equation, namely

$$[-\frac{1}{2}\nabla_{\mathbf{r}}^2 - \frac{1}{2}k^2]\varphi_{k_{i,v,v_t}}^{(+)}(\mathbf{r}) + \int d\mathbf{r}' \langle \mathbf{r} | V_{\text{opt}} | \mathbf{r}' \rangle \varphi_{k_{i,v,v_t}}^{(+)}(\mathbf{r}') = 0. \quad (20.201)$$

It is a simple matter to verify that the presence of the term  $\langle \mathbf{r} | V_{\text{orth}} | \mathbf{r}' \rangle$  in eq. (20.199) implies that  $\varphi_{k_{i,v,v_t}}^{(+)}$  is orthogonal to each of the Hartree-Fock orbitals  $\varphi_j$ , as it should be.

(ii) Another way of obtaining an approximate expression for the second order term  $V^{(2)}$  given by eq. (20.190) may be obtained as follows [44-45]. Let us introduce a complete set of plane waves to write a matrix element  $\langle \mathbf{r} | V^{(2)} | \mathbf{r}' \rangle$  of  $V^{(2)}$  as

$$\langle \mathbf{r} | V^{(2)} | \mathbf{r}' \rangle = \sum_{n \neq 0} \int d\mathbf{k} \langle \mathbf{r} | \mathbf{k} \rangle \frac{\langle 0 | V_d | n \rangle \langle n | V_d | 0 \rangle}{k^2/2M - \kappa^2/2M - (w_n - w_0) + i\varepsilon} \langle \mathbf{k} | \mathbf{r}' \rangle$$

or

$$\begin{aligned} \langle \mathbf{r} | V^{(2)} | \mathbf{r}' \rangle = & -(2\pi)^{-3} \sum_{n \neq 0} \int d\mathbf{k} \exp\{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')\} \\ & \times \frac{\langle 0 | V_d | n \rangle \langle n | V_d | 0 \rangle}{\kappa^2/2M - k^2/2M - (w_0 - w_n) - i\varepsilon}. \end{aligned} \quad (20.202)$$

At sufficiently high colliding energies it is reasonable to replace the differences  $w_n - w_0$  by an *average excitation energy*  $\bar{w}$  [46]. In this case we may perform the sum on  $n$  by closure so that

$$\begin{aligned} \langle \mathbf{r} | V^{(2)} | \mathbf{r}' \rangle = & 2M \left[ - (2\pi)^{-3} \int d\mathbf{k} \frac{\exp\{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')\}}{\kappa^2 - \bar{k}^2 - i\varepsilon} \right] \\ & \times [\langle 0 | V_d^2 | 0 \rangle - \langle 0 | V_d | 0 \rangle \langle 0 | V_d | 0 \rangle] \end{aligned} \quad (20.203a)$$

with

$$\bar{k} = (k^2 - 2M\bar{w})^{1/2}. \quad (20.203b)$$

The first bracket in eq. (20.203a) is easily recognized as the free Green's function  $G_0^{(+)}(\bar{k}, \mathbf{r}, \mathbf{r}')$  corresponding to the wave number  $\bar{k}$ . Furthermore, if we define the object

$$A(\mathbf{r}, \mathbf{r}') = 2M[\langle 0 | V_d^2 | 0 \rangle - \langle 0 | V_d | 0 \rangle \langle 0 | V_d | 0 \rangle]$$

or explicitly

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}') = & 2M \left\{ \int |\psi_0(X)|^2 V_d(\mathbf{r}, X) V_d(\mathbf{r}', X) dX \right. \\ & \left. - \left[ \int |\psi_0(X)|^2 V_d(\mathbf{r}, X) dX \right] \left[ \int |\psi_0(X)|^2 V_d(\mathbf{r}', X) dX \right] \right\} \end{aligned}$$



where the symbol  $X$  denotes the target coordinates, we may write the Schrödinger equation for  $\varphi_{k_i, v, v_t}^{(+)}$  as

$$\left[ K + V^{(1)}(\mathbf{r}) - \frac{k^2}{2M} \right] \varphi_{k_i, v, v_t}^{(+)}(\mathbf{r}) + \int d\mathbf{r}' G_0^{(+)}(\mathbf{r}, \mathbf{r}') A(\mathbf{r}, \mathbf{r}') \varphi_{k_i, v, v_t}^{(+)}(\mathbf{r}') = 0. \quad (20.204)$$

Detailed studies of eq. (20.204) have been made, first within the framework of the eikonal approximation [44, 45, 47] and more recently by using the partial-wave method to perform a full-wave treatment [48]. We shall give here an outline of the results obtained for the particular case of the elastic scattering of fast *electrons* by atoms (so that  $M = 1$  and  $Q = -1$ ). As we have already shown above [see the discussion following eq. (20.189)] the static potential  $V^{(1)}$ , which is real and of short range, is dominant at short distances, where it reduces to the Coulomb interaction  $-Z/r$  acting between the projectile electron and the nucleus of the target atom. Therefore, at intermediate and high energies, we should expect the static potential to govern the *large angle* (direct) scattering.

Although the expression (20.203a) for the second order part of the potential is non-local, a careful analysis shows that  $V^{(2)}$  can be approximated by a complex, local potential containing two terms, namely

$$V^{(2)} = V_{\text{pol}} + i V_{\text{abs}}. \quad (20.205)$$

Here the first term  $V_{\text{pol}}$  (which is real) accounts for the *polarization* of the target by the incident particle while the second term (which is imaginary) arises from the *absorption* effects induced by unitarity because of the open channels (i.e. due to the fact that at the energies considered here non-elastic processes can occur). The term  $V_{\text{pol}}$  is dominant at large distances where it is given by [47]

$$V_{\text{pol}}(r) = -\frac{\bar{\alpha}}{2r^4} \left( 1 + \frac{6a^2}{r^2} + \frac{135a^4}{r^4} + \dots \right) \quad (20.206)$$

where  $\bar{\alpha}$  is the dipole polarizability of the atom (obtained in the closure approximation) and  $a = k/2\bar{\omega}$ . It is worth noting that at large distances  $V_{\text{pol}}$  lies *below* the asymptotic form  $-\bar{\alpha}/2r^4$ . This is in contrast with the result which would be obtained from a Buckingham potential of the form given by eq. (20.197).

The absorption potential  $V_{\text{abs}}$  appearing in eq. (20.205) may be obtained by using the Glauber method, together with the work of Joachain and Mittleman [44, 45]. It should be stressed that both polarization and absorption effects are important at *small* angles. This is easy to understand since

- (i)  $V_{\text{pol}}$  is a *long-range* interaction.

(ii) At high energies *non-elastic* processes dominate the total (complete) cross section and hence the imaginary part of the forward elastic scattering amplitude.

Finally, *exchange* effects may be accounted for by using a pseudopotential  $V_{\text{opt}}^{\text{ex}}$  [36]. The full (second order) optical potential then reads

$$V_{\text{opt}} = V^{(1)} + V_{\text{pol}} + i V_{\text{abs}} + V_{\text{opt}}^{\text{ex}}. \quad (20.207)$$

With the optical potential determined in this way, it is now a simple matter to perform a partial wave analysis of the corresponding Schrödinger equation. We show in Fig. 20.6 the results obtained for the elastic scattering

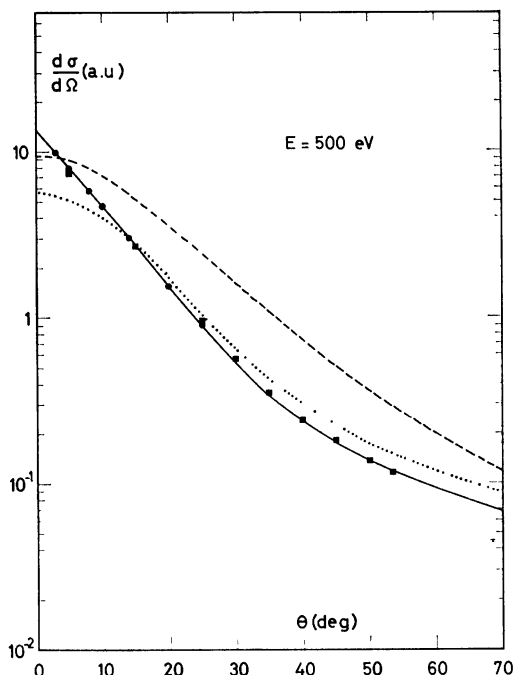


Fig. 20.6. Differential cross section (in atomic units  $a_0^2/\text{sr}$ ) for elastic electron-neon scattering at an incident electron energy of 500 eV. *Solid line*: Optical model calculation, using an average excitation energy of  $\bar{\omega} = 1.5$  a.u. [48]; *Dotted line*: static potential only; *Dashed line*: first Born approximation. The dots are the experimental results of Bromberg [50]; the squares correspond to the experimental data of Jansen *et al.* [51].

of electrons by neon, at an incident electron energy of 500 eV. The wave function describing the ground state of the neon atom was chosen to be a Hartree-Fock wave function [49]. The solid curve represents the optical model curve, obtained by using an average excitation energy  $\bar{\omega} = 1.5$  a.u. [48]. This value is determined by requiring that the quantity  $\bar{\alpha}$  appearing in eq. (20.206) should be the experimental dipole polarizability of the target atom. The dotted curve shows the results obtained by using only the static potential

$V^{(1)}$  and the dashed curve represents the values obtained from the first Born approximation. The dots and squares refer to the experimental data [50, 51].

It is clear from the examination of Fig. 20.6 that the static potential – treated “exactly” by means of the partial-wave method – gives a good description of the scattering outside the small angle region. At small momentum transfers the second order terms in the optical potential yield an important contribution to the scattering, while exchange effects are relatively small at the energy and angles considered in Fig. 20.6. It is also interesting to note the large difference between the first Born and optical model results, even at this rather high (atomic) energy. The optical model curve, which includes the static potential and the polarization, absorption and exchange effects is seen to be in excellent agreement with the experimental values. Finally, it is worth remarking that the small angle region over which the polarization and absorption effects are important becomes more and more narrow as the incident electron energy increases. At very large (non-relativistic) energies the first Born amplitude (which is proportional to the Fourier transform of the static potential) eventually describes correctly the elastic scattering for all angles.

#### 20.4.2. *Low energy electron–atomic hydrogen resonance scattering*

We shall now apply the Feshbach projection operator formalism of Section 20.2.3 to analyze the low energy resonance scattering of electrons by hydrogen atoms. Before we do so, however, let us look at the physics of the situation. Suppose for a moment that the electron–electron interaction of the ( $e^- + H$ ) system has been turned off. The spectrum of the system  $p + e^- + e^-$  is then given by Fig. 20.7, where we have denoted by  $(\alpha, \alpha')$  the quantum numbers of the two electrons. We see that apart from the ground state  $(1s, 1s)$ , there are an infinite number of bound states between the level  $(1s, 2s)$  and the first ionization limit  $(1s, k')$  where one of the electrons becomes free and the remaining hydrogen atom is left in its ground state (principal quantum number  $n = 1$ ). Higher up in energy, there are again an infinite number of bound states, embedded in the  $(1s, k')$  continuum and extending to the second ionization limit  $(2s, k')$ , where the remaining hydrogen atom is left in the excited state with principal quantum number  $n = 2$ . If we still increase the energy, we find similar sequences of bound states embedded in the continuum, and extending to the third, fourth, etc. ionization limits (with the remaining hydrogen atom left in excited states with  $n = 3, 4, \dots$ ). Finally, the “pure” continuum region begins when the total energy  $E$  of the ( $e^- + H$ ) system vanishes, corresponding to the fact that the two electrons are free.

We now switch on the electron–electron interaction. Then among the infinite number of bound states lying between the levels  $(1s, 1s)$  and the first ionization threshold  $(1s, k')$  it is known that only *one* survives, namely the

$^1S_0$  ground state of the hydrogen negative ion  $H^-$ . Given that there is one bound state remaining below  $(1s, k')$  when the electron–electron interaction is taken into account, it is interesting to ask if any “bound states” remain in the continuum between  $(1s, k')$  and  $(2s, k')$  when the electron–electron interaction is turned on. This region of energy, lying above the first ionization threshold but below the second one is precisely the *elastic scattering region*. Evidently, any “bound state” here would actually be unstable against the ejection of an electron, with the other electron falling back to the ground

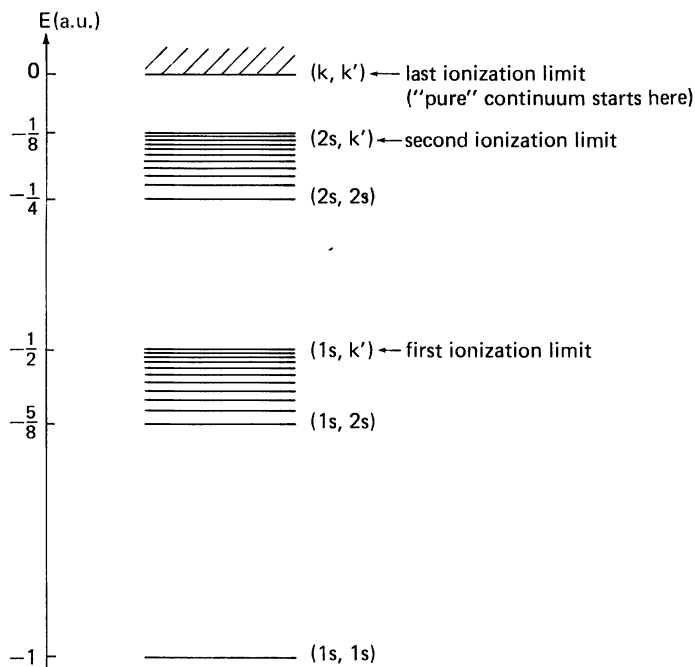


Fig. 20.7. The spectrum of the  $(e^- + H)$  system in the absence of electron–electron interaction.

state  $(1s)$  of the remaining hydrogen atom. For this reason such “bound states” are called *auto-ionizing states*. Thus, just as the interaction of the electromagnetic field with matter produces unstable excited bound states with a width in energy, so will the electron–electron interaction give a width to any “bound state” embedded in the  $(1s, k')$  continuum. We should therefore expect that any incident electron having an energy falling within the width of such auto-ionizing states will spend a long time in the vicinity of the atom, thus giving rise to a *resonance* in the scattering cross section [52].

We are now prepared to apply the Feshbach projection operator formalism in order to investigate electron–atomic hydrogen resonance scattering below

the first inelastic threshold. We first write the Schrödinger equation for the  $(e^-, H)$  system as

$$(H - E)\Psi(r_1, r_2) = 0 \quad (20.208)$$

where the Hamiltonian operator of the system is given by

$$H = -\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} \quad (20.209)$$

and the wave function  $\Psi$  is also an eigenfunction of the total operators  $L^2$ ,  $L_z$  and parity of the two-electron system. Since we have only displayed the spatial coordinates  $r_1$  and  $r_2$  of the two electrons in the wave function  $\Psi$ , we require  $\Psi$  to be symmetric for singlet states and antisymmetric for triplet states in order to satisfy the Pauli principle. The asymptotic form of  $\Psi$  for the case of scattering below the inelastic threshold and for (say)  $r_2 \rightarrow \infty$  may be chosen (using an angular momentum representation) to be

$$\Psi(r_1, r_2) \xrightarrow{r_2 \rightarrow \infty} [\sin(kr_2 - \frac{1}{2}L\pi + \delta_l)/kr_2] Y_{LM}(\hat{r}_2) \psi_{1s}(r_1) \quad (20.210)$$

where  $\psi_{1s}$  is the hydrogen atom ground state wave function.

We now construct the two projection operators  $P$  and  $Q$  of the Feshbach method which permit one to separate the scattering problem into a ground state sector and an excited state sector. Following Hahn, O'Malley and Spruch [53], we first write the  $Q$ -operator as

$$Q = Q_1 Q_2 \quad (20.211)$$

with

$$Q_i = 1 - P_i \quad (i = 1, 2). \quad (20.212)$$

Here

$$P_i = |\psi_{1s}(r_i)\rangle\langle\psi_{1s}(r_i)| \quad (20.213)$$

is the operator which projects out the hydrogenic ground state in the  $i$ th electron coordinate. The  $P$  operator is then given by

$$P = 1 - Q. \quad (20.214)$$

It is a simple matter to verify that the  $P$  and  $Q$  operators defined above (which are symmetric in  $r_1$  and  $r_2$ ), satisfy the requirements of the Feshbach method, namely

$$P + Q = 1, \quad P^2 = P, \quad Q^2 = Q \quad (20.215)$$

and

$$P\Psi \xrightarrow{r_1 \text{ or } r_2 \rightarrow \infty} \Psi. \quad (20.216)$$

The second important step in the Feshbach method is to solve eq. (20.119), namely

$$H_{QQ}\chi_v = \varepsilon_v \chi_v.$$

Since  $Q\chi_v = \chi_v$ , we can write

$$\varepsilon_v = \frac{\langle\chi_v|QHQ|\chi_v\rangle}{\langle\chi_v|\chi_v\rangle} = \frac{\langle Q\chi_v|H|Q\chi_v\rangle}{\langle Q\chi_v|Q\chi_v\rangle}. \quad (20.217)$$

TABLE 20.1.

Calculated positions of some resonances occurring in the compound system ( $e^- + H$ ) below the energy of the 2s state of H (at 10.204 eV). All energies are measured up from the ground state of H (taken from ref. [54]).

Type of resonance	Energy (eV)
$^1S$	9.559
$^3P$	9.727
$^3S$	10.149
$^1S$	10.178
$^1P$	10.178
$^3P$	10.198
$^3S$	10.202
$^1P$	10.203

Therefore, if we construct trial functions of the form  $Qf$ , we have a variational principle for the discrete eigenvalues  $\varepsilon_n$ , with a minimum principle for the lowest value. The variational calculation of the spectrum of the operator  $QHQ$  has been carried out by O'Malley and Geltman [54], using the Rayleigh-Ritz variational method.

We now return to eq. (20.140) which describes resonant scattering in the Feshbach formalism. Careful investigation shows that the quantities  $\Delta_n$  and  $\Gamma_n$  are very small compared to the spacing between low-lying resonances. The values of  $\varepsilon_n$  obtained from eq. (20.217) therefore give a good approximation of the resonance energies. For example, we list in Table 20.1 the positions of resonances (i.e. the values of  $\varepsilon_n$ ) found by O'Malley and Geltman [54] who investigated the states  $^1S$ ,  $^3S$ ,  $^1P$  and  $^3P$ . Similar calculations done by these authors for the system ( $e^- - He^+$ ) also yield a variety of resonances, some of which have been observed experimentally [55].

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- [11] A comprehensive review of the optical potential method, including applications which are not discussed here, may be found in FETTER, A. L. and K. M. WATSON (1965), in *Advances in Theoretical Physics*, ed. K. A. Brueckner (Academic Press, New York) Vol. 1, p. 115.
- [12] Note that we are including here the spin-flip transitions among the "elastic" scattering processes. In what follows we shall often omit the spin indices and write  $\psi_0$  for the target bound state wave function.
- [13] For example, if the target is an atom having  $N$  electrons, the Hartree-Fock method provides convenient ground state wave functions  $\psi_0$ .
- [14] It is apparent that  $\mathcal{T}_c$  and  $T_c$  are  $(2S+1)(2S_t+1) \times (2S+1)(2S_t+1)$  matrices in spin space. We shall assume in what follows that the only degeneracies which are present are those corresponding to the spin orientation. Other kinds of degeneracies, such as those associated with the isospin, may easily be included by generalizing the notation adopted here.
- [15] Of course the full many-body interaction  $V_d$  given by eq. (20.18) must be an Hermitian operator, since we require the total Hamiltonian  $H$  to be Hermitian from total probability conservation.
- [16] We note that eq. (20.62) is not restricted to non-relativistic collisions, so that it generalizes eq. (9.30) of Section 9.1.
- [17] Since the Hamiltonian  $H_d$  given by eq. (20.12) includes the internal Hamiltonian of the target, the Green's operator  $G_d^{(+)}$  introduced here should not be confused with the "totally free" Green's operator  $G_0^{(+)}$ .
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- [22] This is the case when the collision between the incident particle and a target particle may lead to several final channels. For example, a pion incident on a target nucleus may react with a target nucleon  $N$  as:  $\pi + N \rightarrow \pi + N$   
 $\rightarrow A_1 + N$   
 $\rightarrow 3\pi + N$ , etc.
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 [26] We note that the approximate expression (20.171) of  $\chi_{\text{opt}}$  in the impulse approximation is such that

$$\exp(i\chi_{\text{opt}}(\mathbf{b})) \simeq 1 + A \frac{2\pi i}{k_L} f_L(0) \int_{-\infty}^{+\infty} \rho(\mathbf{b}, z) dz$$

so that

$$f_{\text{el}}^{\text{IA}} = A f_L(0) \int d^2\mathbf{b} \exp(i\mathbf{q} \cdot \mathbf{b}) \int_{-\infty}^{+\infty} dz \rho(\mathbf{b}, z); \quad \mathbf{q} = \mathbf{k}_L - \mathbf{k}_L'$$

and

$$d\sigma_{\text{el}}^{\text{IA}}/d\Omega = A^2 |f_L(0)|^2 |S(\mathbf{q})|^2 = A^2 (d\sigma(0)/d\Omega) |S(\mathbf{q})|^2$$

with

$$S(\mathbf{q}) = \int \exp(i\mathbf{q} \cdot \mathbf{r}) \rho(\mathbf{r}) d\mathbf{r}.$$

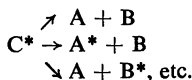
We verify again that in the forward direction the impulse approximation cross section is such that  $d\sigma_{\text{el}}^{\text{IA}}/d\Omega = A^2 (d\sigma/d\Omega)_f$ .

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 [39] We recall that when the target atom is an hydrogen atom in its ground state we found in Section 19.5 for the case of incident electrons [see eq. (19.158)] that  

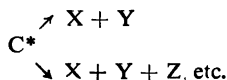
$$V^{(1)}(\mathbf{r}) = V_{\text{st}}(\mathbf{r}) = \langle 0 | V_d | 0 \rangle = -(1 + 1/r) \exp(-2r).$$



- [40] We recall in this connection that inelastic transitions corresponding to "allowed" transitions in the target atom dominate at high energies (see for example the calculation of Section 19.5.2 for the "allowed" transition  $1s \rightarrow 2p$  in atomic hydrogen induced by electron impact, where we showed that the total cross section for this process behaves at high energies like  $(\log E_e)/E_e$  while the total elastic cross section is only proportional to  $E_e^{-1}$ ).
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- [52] This resonance process may be written as  $e^- + H(1s) \rightarrow H^{-*} \rightarrow e^- + H(1s)$ , where  $H^{-*}$  is a metastable state of the  $H^-$  ion. It is a particular case of a resonance occurring in a "formation" experiment. In such experiments the two colliding particles A and B first combine to form a long-lived complex  $C^*$  which subsequently decays. Thus one first has  $A + B \rightarrow C^*$  and then



It is also possible to obtain resonances in "production" experiments. Here the resonance is produced together with other particles during the reaction. Hence one first has for example  $A + B \rightarrow C^* + D$  and then



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## Topics in Multiparticle Collisions

In this chapter we shall analyze a few typical multiparticle collision processes. We begin in Section 21.1 by considering electron–helium scattering. Nuclear stripping and pick-up reactions are studied in Section 21.2. Section 21.3 is devoted to the theory of final state interactions, which we illustrate by analyzing the photoelectric effect in atoms.

### 21.1. *Electron–helium collisions*

The scattering of electrons by atoms is one of the most important problems in atomic collision theory. The case of electron collisions with atomic hydrogen was studied in some detail in Section 19.5, and we have shown in Section 20.4 how to construct an optical potential describing the elastic scattering of charged particles by atoms. In this section we shall focus our attention on electron–helium collisions, for which “a priori” calculations can still be done with a reasonable amount of computational effort, and good experimental data are available. In particular, we shall analyze in some detail *elastic* electron–helium scattering at intermediate and high (atomic) energies,

#### 21.1.1. *Preliminaries*

Let us denote respectively by  $\mathbf{r}_0$ ,  $\mathbf{r}_1$  and  $\mathbf{r}_2$  the coordinates of the “incident” and of the two “atomic” electrons (in the initial channel) with respect to the alpha particle (which we assume to be infinitely heavy). We neglect all but the Coulomb interactions between the particles and assume that the helium atom is initially in the ground state  $1^1\text{S}$ , described by the wave function

$$\Psi_0(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = \psi_0(\mathbf{r}_1, \mathbf{r}_2) \chi_{S=0, v=0}(s_1, s_2) \quad (21.1)$$

where  $\psi_0(\mathbf{r}_1, \mathbf{r}_2)$ , the spatial part of the wave function, is symmetric under the interchange of  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , while

$$\chi_{S=0, v=0}(s_1, s_2) = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \alpha(2)\beta(1)]. \quad (21.2)$$

The incident free electron, having a wave vector  $\mathbf{k}_i$  and a spin orientation  $v_0$  is described by the wave function (19.124), namely

$$\phi_{\mathbf{k}_i, v_0} = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \chi_{v_0}(s_0) \quad (21.3)$$

so that the complete unsymmetrized free wave describing the initial state is given by

$$\Phi_a = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_0(\mathbf{r}_1, \mathbf{r}_2) \chi_{v_0}(s_0) \chi_{S=0, v=0}(s_1, s_2). \quad (21.4)$$

For example, if the incident electron has initially "spin up", we have

$$\Phi_a = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_0) \psi_0(\mathbf{r}_1, \mathbf{r}_2) \alpha(0) \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \alpha(2)\beta(1)]. \quad (21.5)$$

The free wave  $\Phi_a$  is evidently an eigenvector of the initial arrangement channel Hamiltonian

$$H_i = -\frac{1}{2}\nabla_{\mathbf{r}_0}^2 - \frac{1}{2}\nabla_{\mathbf{r}_1}^2 - \frac{1}{2}\nabla_{\mathbf{r}_2}^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \quad (21.6)$$

where we have used atomic units (a.u.) [1]. The complete Hamiltonian of the system is given by

$$H = -\frac{1}{2}\nabla_{\mathbf{r}_0}^2 - \frac{1}{2}\nabla_{\mathbf{r}_1}^2 - \frac{1}{2}\nabla_{\mathbf{r}_2}^2 - \frac{2}{r_0} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{01}} + \frac{1}{r_{02}} + \frac{1}{r_{12}} \quad (21.7)$$

so that the interaction potential in the initial arrangement channel is

$$V_i = \frac{1}{r_{01}} + \frac{1}{r_{02}} - \frac{2}{r_0}. \quad (21.8)$$

As in the case of electron scattering by atomic hydrogen (see Section 19.5) we must consider both *direct* and *exchange* collisions. For direct scattering the interaction  $V_d = V_i = V_f$  is the same in the initial and final arrangement channels. On the contrary, for an exchange collision in which, say, the electrons "0" and "1" exchange their role, the interaction potential in the final arrangement channel is given by

$$V_{P(01)} = \frac{1}{r_{01}} + \frac{1}{r_{12}} - \frac{2}{r_1} \quad (21.9)$$

where  $P_{(01)}$  means that we interchange the electrons "0" and "1".

According to the general equation (16.160) the correctly symmetrized transition matrix element describing a process  $a \rightarrow b$  reads in this case

$$\bar{T}_{ba} = T_{ba}^d - 2T_{ba}^{ex} \quad (21.10)$$

where the direct transition matrix element is such that

$$T_{ba}^d = \langle \Phi_b | V_d | \Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)} | V_d | \Phi_a \rangle \quad (21.11)$$

while the exchange matrix element is given by

$$T_{ba}^{ex} = \langle \Phi_{P(01)b} | V_{P(01)} | \Psi_a^{(+)} \rangle = \langle \Psi_{P(01)b}^{(-)} | V_d | \Phi_a \rangle \quad (21.12)$$

[see eqs. (19.138)–(19.139)]. The reduction of the spin parts of the matrix elements (21.11) and (21.12) can be done as in Section 19.5. Calling  $\hat{T}_{ba}^d$  and  $\hat{T}_{ba}^{ex}$  the corresponding reduced transition matrix elements one finds that for transitions leading to final *singlet* helium states, the differential cross section is given by

$$\frac{d\sigma}{d\Omega}(\text{singlet}) = (2\pi)^4 \frac{k_f}{k_i} |\hat{T}_{ba}^d - \hat{T}_{ba}^{ex}|^2 \quad (21.13a)$$

or, in terms of the direct scattering amplitude  $f_{ba} = -(2\pi)^2 \hat{T}_{ba}^d$  and the exchange scattering amplitude  $g_{ba} = -(2\pi)^2 \hat{T}_{ba}^{ex}$ , one has

$$\frac{d\sigma}{d\Omega}(\text{singlet}) = \frac{k_f}{k_i} |f_{ba} - g_{ba}|^2. \quad (21.13b)$$

For transitions leading to *triplet* states, one obtains instead

$$\frac{d\sigma}{d\Omega}(\text{triplet}) = (2\pi)^4 \frac{3k_f}{k_i} |\hat{T}_{ba}^{ex}|^2 \quad (21.14a)$$

or

$$\frac{d\sigma}{d\Omega}(\text{triplet}) = \frac{3k_f}{k_i} |g_{ba}|^2. \quad (21.14b)$$

We note that if we neglect very small spin-dependent interactions, the excitation of a triplet state of helium by electron bombardment can only occur through exchange between the projectile electron and one of the initially bound electrons. This process is therefore one of the simplest examples of a “pure” rearrangement collision (of the “knock-out” type) in atomic physics.

### 21.1.2. Elastic scattering of fast electrons by helium

Let us now consider in more detail the elastic scattering of “fast” electrons (having an energy somewhat larger than 100 eV) by helium atoms. We shall use for  $\psi_0(\mathbf{r}_1, \mathbf{r}_2)$  a simple analytical fit to the Hartree–Fock ground state wave function, namely [2]

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \phi_0(r_1)\phi_0(r_2) \quad (21.15a)$$

with

$$\phi_0(x) = (4\pi)^{-1/2} (Ae^{-\alpha x} + Be^{-\beta x}) \quad (21.15b)$$

and  $A = 2.60505$ ,  $B = 2.08144$ ,  $\alpha = 1.41$  and  $\beta = 2.61$ . With this wave

function the reduction of the second Born direct amplitude is analogous to that discussed above in the case of atomic hydrogen (see Section 19.5.3). Similarly, the Glauber expression  $\bar{f}_{G3}$  [see eq. (19.121)] can also be evaluated in this case, so that the direct elastic amplitude may be written (through terms of order  $k^{-2}$ ) as [see eq. (19.208)]

$$f_{el}^d = f_{B1} + \text{Re } \bar{f}_{B2} + \bar{f}_{G3} + i \text{Im } \bar{f}_{B2}. \quad (21.16)$$

The leading term  $g_{el}^{\text{Och}}$  of the exchange amplitude (which is of order  $k^{-2}$ ) may also be evaluated as in the case of electron–hydrogen collisions by using a straightforward generalization of the Ochkur expression (19.191), namely

$$g_{el}^{\text{Och}} = -(2\pi)^2 T_{el}^{\text{Och}} \quad (21.17)$$

where

$$T_{el}^{\text{Och}} = \frac{1}{2\pi^2 k^2} \int \exp(i\mathbf{A} \cdot \mathbf{r}_1) |\psi_0(\mathbf{r}_1, \mathbf{r}_2)|^2 d\mathbf{r}_1 d\mathbf{r}_2. \quad (21.18)$$

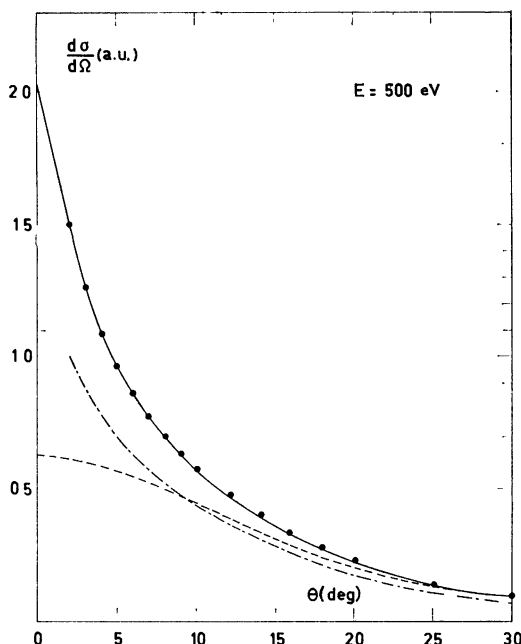


Fig. 21.1. The differential cross section (in atomic units  $a_0^2/\text{sr}$ ) for elastic scattering of electrons by helium at 500 eV. The solid curve refers to the eikonal-Born series results obtained by using eq. (21.20) of the text (ref. [4]). The dashed curve corresponds to the first Born approximation, and the dashed-dotted curve refers to the Glauber approximation. The circles are the absolute experimental results of ref. [5].

Using the Hartree-Fock wave function (21.15), one finds

$$g_{\text{el}}^{\text{Och}} = -\frac{8}{k^2} \left[ \frac{\alpha A^2}{(4\alpha^2 + \Delta^2)^2} + \frac{(\alpha + \beta)AB}{((\alpha + \beta)^2 + \Delta^2)^2} + \frac{\beta B^2}{(4\beta^2 + \Delta^2)^2} \right] \quad (21.19)$$

where  $\Delta$  is the magnitude of the momentum transfer. Using eq. (21.13b), we may therefore write the *eikonal-Born series* (EBS) elastic differential cross section (through terms of order  $k^{-2}$ ) as

$$\frac{d\sigma_{\text{el}}}{d\Omega} = |f_{\text{el}}^{\text{d}} - g_{\text{el}}^{\text{Och}}|^2 \quad (21.20)$$

where the quantities  $f_{\text{el}}^{\text{d}}$  and  $g_{\text{el}}^{\text{Och}}$  are given respectively by eqs. (21.16) and (21.19).

As in the case of the elastic scattering of electrons by atomic hydrogen [3], we expect that the EBS expression (21.20) should be very accurate for large  $k$  and small momentum transfers, in which case the Born series for  $f_{\text{el}}^{\text{d}}$  is converging rapidly and the term  $g_{\text{el}}^{\text{Och}}$  provides the leading exchange correction. This is illustrated in Fig. 21.1, where we show the EBS results [4] obtained from eq. (21.20), together with small angle absolute experimental data [5], at an incident electron energy of 500 eV. Also shown on Fig. 21.1 are the results

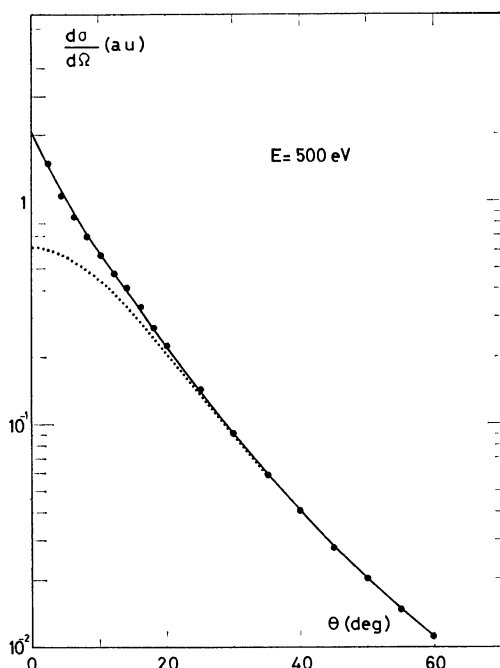


Fig. 21.2. The differential cross section (in atomic units  $a_0^2/\text{sr}$ ) for elastic scattering of electrons by helium at 500 eV. The solid curve refers to the eikonal Born-series results of ref. [6]. The dotted curve corresponds to an exact (partial wave) treatment of the static potential  $V_{\text{st}}$ . The circles show the absolute experimental data of ref. [5].

given by the first Born approximation and those corresponding to the Glauber approximation (i.e.  $d\sigma_{el}^G/d\Omega = |f_{el}^G|^2$ , with  $f_{el}^G$  obtained from eq. 19.118). It may be seen from Fig. 21.1 that the eikonal-Born series results are in excellent agreement with experiment. The Glauber differential cross section which diverges in the forward direction and lacks the terms  $\text{Re } \tilde{f}_{B2}$  and  $g_{el}^{\text{Och}}$  is seen to be deficient. We also remark that even at 500 eV the first Born differential cross section is still very inaccurate at small angles, although at sufficiently high (non-relativistic) energies it eventually describes correctly this elastic scattering process.

At high energies and large momentum transfers we expect that the static potential  $V_{st} = \langle 0|V_d|0 \rangle$  will govern the scattering. This is confirmed by a careful analysis of higher terms of the Born and Glauber series [6]. As an illustration, we display in Fig. 21.2 the results obtained by solving numerically the partial wave radial equations corresponding to the static potential  $V_{st}$ , together with absolute experimental data [5]. Also shown for comparison are the EBS values obtained from eq. (21.20). We note from Fig. 21.2 that the static and EBS results agree very well with each other and with the experimental results outside the small angle region [7]. At small angles the EBS results are seen to be more accurate, as we expect from the above discussion.

### 21.1.3. Forward dispersion relations

We have shown in Chapter 11 that for a large class of central potentials the forward scattering amplitude is analytic as a function of the energy, except for poles occurring at the bound state energies and a cut extending along the real energy axis [see eq. (11.228)]. It is then possible to write a forward dispersion relation of the form (11.229), namely

$$\text{Re } f(E) = f_{B1} + \sum_{i=1}^N \frac{\tilde{R}_i}{E - E_i} + \frac{P}{\pi} \int_0^\infty \frac{\text{Im } f(E')}{E' - E} dE' \quad (21.21)$$

where  $f(E) \equiv f(\theta = 0, E)$  denotes the scattering amplitude in the forward direction,  $f_{B1}$  is the first Born amplitude and  $\tilde{R}_i$  are the “residues” of the poles at  $E = E_i$ .

Let us now *assume* that such forward dispersion relations still hold for elastic electron-atom scattering [8]. Using this assumption, Lawson *et al.* [9] have analyzed elastic electron-helium collisions. In this case no bound state of  $\text{He}^-$  exist and the assumed generalization of eq. (21.21) (taking into account exchange effects) reads

$$\text{Re } f_{el}(\theta = 0, E_e) = f_{B1}(\theta = 0) - g_{B1}(\theta = 0, E_e) + \frac{P}{\pi} \int_0^\infty \frac{\text{Im } f_{el}(\theta = 0, E')}{E' - E_e} dE' \quad (21.22)$$

where  $E_e$  is the incident electron energy,  $f_{el}(\theta = 0, E_e)$  is the forward elastic scattering amplitude (including exchange effects),  $f_{B1}$  is the first Born

approximation for the direct amplitude (which is independent of  $E_e$ ) and  $g_{B1}$  is the first Born approximation for the exchange amplitude, namely

$$g_{B1} = -(2\pi)^{-1} \int \exp(-ik_f \cdot r_1) \psi_0(r_0, r_2) \left[ \frac{1}{r_{01}} + \frac{1}{r_{02}} - \frac{2}{r_0} \right] \times \exp(ik_i \cdot r_0) \psi_0(r_1, r_2) dr_0 dr_1 dr_2. \quad (21.23)$$

The point  $\theta = 0$  is of course not directly accessible to experiments, since elastic differential cross sections cannot be measured in the forward direction. However, if we combine the dispersion relation (21.22) with the generalized optical theorem (15.176), namely

$$\text{Im } f_{el}(\theta = 0, E_e) = \frac{\sqrt{2E_e}}{4\pi} \sigma_{tot}(E_e) \quad (21.24)$$

we find that

$$\text{Re } f_{el}(\theta = 0, k) = f_{B1}(\theta = 0) - g_{B1}(\theta = 0, k) + \frac{1}{2\pi^2} P \int_0^\infty \frac{k'^2 \sigma_{tot}(k')}{k'^2 - k^2} dk' \quad (21.25)$$

where we have used the fact that  $E_e = \frac{1}{2}k^2$  (in atomic units). Therefore, if values of the total (complete) cross section  $\sigma_{tot}$  are known for all energies (or wave numbers), then  $\text{Re } f_{el}(\theta = 0, E_e)$  can be obtained for any energy. Since  $\text{Im } f_{el}(\theta = 0, E_e)$  is known from the optical theorem (21.24), the forward elastic differential cross section  $d\sigma_{el}(\theta = 0)/d\Omega$  can then be evaluated and compared with the "experimental" values obtained by extrapolating small angle elastic scattering differential cross sections down to  $\theta = 0$ .

Detailed calculations of this kind have been carried out for helium by Bransden and McDowell [10]. At low energies ( $k \leq 1.2$  a.u.) they used the total cross section measurements of Golden and Bandel [11]. At high energies ( $k \geq 4.5$  a.u.) they obtained the total (complete) cross section by writing

$$\sigma_{tot} \simeq \sigma_{tot}^{el}(\text{Born}) + \sigma_{tot}^{inel}(\text{Born}) \quad (21.26)$$

and using the first Born values of Kennedy [12] for  $\sigma_{tot}^{el}(\text{Born})$  and the Bethe-Born values of Inokuti, Kim and Platzman [13] for  $\sigma_{tot}^{inel}(\text{Born})$ . At intermediate energies (i.e. between the values  $k = 1.2$  and  $k = 4.5$ ) they used a three-term interpolation formula. For energies between 100 eV and 500 eV the results for  $\text{Re } f(\theta = 0, E_e)$  do not depend too sensitively on the region of interpolation, so that the values of  $\text{Re } f(\theta = 0, E_e)$  were estimated by Bransden and McDowell to be accurate to about 15%. The corresponding forward elastic differential cross section was found to be in good agreement at 500 eV with the absolute small angle data of Bromberg [5], extrapolated down to  $\theta = 0$ .

It is interesting to compare the dispersion relation values of  $\text{Re } f_{el}(\theta = 0, E_e)$  [obtained from eq. (21.25)] with various theoretical calculations. As an example, we show in Table 21.1 the dispersion relation results of Bransden



and McDowell [10], together with the corresponding eikonal-Born series [4] quantities  $\text{Re} f_{\text{el}}(\theta = 0, E_e) = \text{Re}[f_{\text{el}}^{\text{d}}(\theta = 0, E_e) - g_{\text{el}}^{\text{Och}}(\theta = 0, E_e)]$  for electron energies ranging from 100 eV to 500 eV. We see that at all energies the EBS and the dispersion relation results agree within the 15% uncertainty quoted above [14].

TABLE 21.1

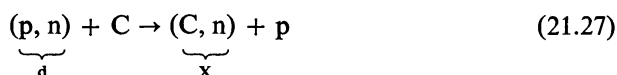
The real part of the forward elastic scattering amplitude for electron-helium collisions, as obtained from dispersion relations [10] and from the eikonal-Born series method [4] at various incident electron energies

$E$ (eV)	$\text{Re} f_{\text{el}}(\theta = 0, E_e)$ (dispersion relations)	$\text{Re} f_{\text{el}}(\theta = 0, E_e) = \text{Re}[f_{\text{el}}^{\text{d}}(\theta = 0, E_e) - g_{\text{el}}^{\text{Och}}(\theta = 0, E_e)]$ (EBS method)
100	1.91	1.91
150	1.81	1.67
200	1.71	1.54
300	1.48	1.39
400	1.36	1.30
500	1.29	1.24

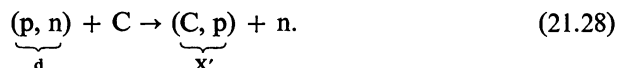
## 21.2. Nuclear stripping and pick-up reactions

### 21.2.1. Preliminaries

Let us consider a deuteron incident on a nucleus C of mass number  $A$ , containing  $Z$  protons and  $N$  neutrons. In a stripping reaction the deuteron loses either its neutron or its proton to the nucleus, so that

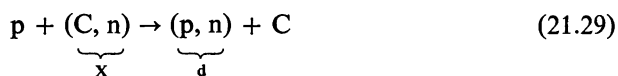


or

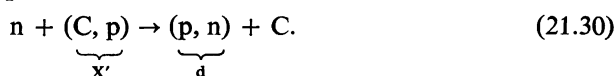


The first reaction (21.27), called the (d, p) stripping process, leads to a final nucleus X containing the core C plus a neutron. The second reaction, denoted as the (d, n) process, yields a final nucleus X' containing the core C plus a proton.

The pick-up reactions are the inverses of the stripping reactions. Thus a (p, d) pick-up process is such that



while a (n, d) pick-up process is written as



It is apparent that the stripping and pick-up reactions (21.27)–(21.30) are binary rearrangement collisions, which we may consider approximately as “three-body problems”, provided the many-body structure of the core C is not taken into account. It is also clear that the reactions (21.27)–(21.28) are related to (21.29)–(21.30) by time-reversal. Furthermore, since the two stripping reactions (21.27)–(21.28) or pick-up reactions (21.29)–(21.30) are very similar, we shall only study one of these processes, for example the pick-up reaction (21.29). Hence, working in the C.M. system, we consider a non-relativistic proton of incident wave vector  $k_i$  incident on a nucleus X (having a wave vector  $-k_i$ ) made of a core C and an “optical” neutron n. Two particles emerge in the final state: a deuteron of wave vector  $k_f$  and the core C having a wave vector  $-k_f$ .

It will be convenient in what follows to treat the neutrons and the protons separately so that the transition matrix element for the collision will be antisymmetrized separately in the neutron and proton coordinates. For the moment, however, we neglect the effects of the Pauli principle on the collision. The initial arrangement channel Hamiltonian describing the proton and the nucleus  $X = (C, n)$  when they are far apart is given by

$$H_i = K_i + h_i \quad (21.31)$$

where the relative initial kinetic energy operator  $K_i$  is given by

$$K_i = -\frac{\hbar^2}{2M_i} \nabla_{r_i}^2 \quad (21.32)$$

with

$$M_i = MM_X/(M + M_X). \quad (21.33)$$

Here  $M$  is the mass of the nucleon (we neglect the mass difference between the neutron and the proton) and  $M_X$  the mass of the nucleus X. The vector  $r_i$  is the relative initial vector joining the C.M. of the target to the position of the incident proton (see Fig. 21.3). Furthermore, the Hamiltonian  $h_i$  describes the internal state of the target nucleus, with

$$h_i \psi_i(\xi, r_0, s_0) = w_i \psi_i(\xi, r_0, s_0) \quad (21.34)$$

where  $w_i$  is the bound state energy of the target nucleus and  $\psi_i$  its wave function. The symbol  $\xi$  summarizes all the spatial and spin coordinates of the  $Z$  protons and  $N$  neutrons of the core, while  $r_0$  and  $s_0$  are the spatial and

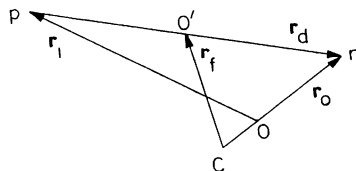


Fig. 21.3. Illustration of the vectors used in the description of the pick-up reaction (21.29). The center of mass of  $(C, n)$  is denoted by O, that of the deuteron  $(p, n)$  is called O'.

spin coordinates of the "optical" neutron (see Fig. 21.3). We shall assume that the wave function  $\psi_i$  has already been antisymmetrized in the coordinates of its  $Z$  protons and  $(N + 1)$  neutrons [15].

If we take into account the fact that the target nucleus  $X$  is made of a core  $C$  and an "optical" neutron  $n$ , we may write the internal Hamiltonian  $h_i$  as

$$h_i = h_c + h_n \quad (21.35)$$

where  $h_c$  is the internal Hamiltonian of the core, such that [16]

$$h_c \psi_c(\xi) = w_c \psi_c(\xi) \quad (21.36)$$

and  $h_n$  is the Hamiltonian of the neutron in the target. Hence, if  $K_n$  and  $V_{nc}$  are respectively the kinetic and potential energies of the optical neutron with respect to the core, we may write

$$h_n \psi_n(\mathbf{r}_0, s_0) = (K_n + V_{nc}) \psi_n(\mathbf{r}_0, s_0) = w_n \psi_n(\mathbf{r}_0, s_0). \quad (21.37)$$

Thus, returning to eq. (21.34), we have

$$\psi_i(\xi, \mathbf{r}_0, s_0) = \mathcal{A} \psi_c(\xi) \psi_n(\mathbf{r}_0, s_0) \quad (21.38)$$

where  $\mathcal{A}$  is an operator which antisymmetrizes the neutron coordinates. Furthermore,

$$w_i = w_c + w_n. \quad (21.39)$$

The initial unsymmetrized free state  $\Phi_a$  (corresponding to an incident proton distinct from those of the nucleus) such that

$$H_i \Phi_a = E_a \Phi_a \quad (21.40)$$

may therefore be written (neglecting long range Coulomb effects between the incident proton and the target nucleus) as

$$\Phi_a = (2\pi)^{-3/2} \exp(i\mathbf{k}_1 \cdot \mathbf{r}_1) \psi_i(\xi, \mathbf{r}_0, s_0) \chi_{1/2, v_p} \quad (21.41)$$

where  $\chi_{1/2, v_p}$  is the spin function of the proton, corresponding to a spin orientation  $v_p$ . Furthermore, the total energy in the initial channel is given by

$$E_a = \hbar^2 k_i^2 / 2M_i + w_i = \hbar^2 k_i^2 / 2M_i + w_c + w_n. \quad (21.42)$$

If we denote by  $V_{pc}$  the interaction of the incoming proton with the core  $C$  and by  $V_{pn}$  its interaction with the optical neutron, we may write the full interaction in the initial channel as

$$V_i = V_{pc} + V_{pn}. \quad (21.43)$$

Let us now consider the situation in the final channel, consisting of a deuteron and the core  $C$ . The final arrangement channel Hamiltonian is

$$H_f = K_f + h_f \quad (21.44)$$

where  $K_f$  is the relative final kinetic energy, given by

$$K_f = - \frac{\hbar^2}{2M_f} \nabla_{r_f}^2 \quad (21.45)$$

$\mathbf{r}_f$  being the relative vector in the final channel – joining the position of the core C to that of the center of mass of the deuteron (see Fig. 21.3) – and

$$M_f = M_d M_C / (M_d + M_C) \quad (21.46)$$

where  $M_d$  and  $M_C$  are respectively the masses of the deuteron and of the core. The internal Hamiltonian  $h_f$  of the final channel is such that

$$h_f = h_C + h_d \quad (21.47)$$

where  $h_C$  and  $h_d$  are respectively the internal Hamiltonians of the core and of the deuteron. Thus

$$h_d \psi_d(\mathbf{r}_d, s_d) = w_d \psi_d(\mathbf{r}_d, s_d). \quad (21.48)$$

Here  $\mathbf{r}_d$  is the internal space coordinate of the deuteron (see Fig. 21.3),  $s_d$  its spin coordinate and its internal energy is  $w_d \simeq -2.23$  MeV. Thus, taking into account eq. (21.36), we have

$$h_f \psi_f(\xi, \mathbf{r}_d, s_d) = w_f \psi_f(\xi, \mathbf{r}_d, s_d) \quad (21.49)$$

with

$$\psi_f(\xi, \mathbf{r}_d, s_d) = \psi_C(\xi) \psi_d(\mathbf{r}_d, s_d) \quad (21.50)$$

and

$$w_f = w_C + w_d. \quad (21.51)$$

The final unsymmetrized [17] free state  $\Phi_b$  satisfying the equation

$$H_f \Phi_b = E_b \Phi_b \quad (21.52)$$

is then given by [18]

$$\Phi_b = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}_f) \psi_C(\xi) \psi_d(\mathbf{r}_d, s_d) \quad (21.53)$$

while the total energy  $E_b$  available in the C.M. system is simply

$$E_b = \hbar^2 k_f^2 / 2M_f + w_f = \hbar^2 k_f^2 / 2M_f + w_C + w_d. \quad (21.54)$$

Upon comparison of eqs. (21.42) and (21.54) we find that conservation of energy implies that

$$\hbar^2 k_i^2 / 2M_i + w_i = \hbar^2 k_f^2 / 2M_f + w_f \quad (21.55)$$

or

$$\hbar^2 k_f^2 / 2M_f = \hbar^2 k_i^2 / 2M_i + Q_{if} \quad (21.56)$$

with

$$Q_{if} = w_i - w_f = w_n - w_d. \quad (21.57)$$

From this last relation we conclude (cf. Section 2.1) that the pick-up reaction (21.29) is *endothermic* ( $Q_{if} < 0$ ) as soon as the binding energy  $|w_n|$  of the optical neutron in the nucleus X exceeds the value 2.23 MeV of the (weak) binding energy  $|w_d|$  of the deuteron.

Finally, the interaction between the deuteron and the core in the final channel is given by

$$V_f = V_{pC} + V_{nC} \quad (21.58)$$

and the complete Hamiltonian for the entire system is

$$H = H_i + V_i = H_f + V_f. \quad (21.59)$$

### 21.2.2. The calculation of the transition matrix

After these preparations we are now ready to look at the dynamics of the pick-up reaction (21.29). The unsymmetrized transition matrix element on the energy-momentum shell is given by [see eqs. (14.157), (14.158) and (14.174)]

$$T_{ba}^d = \langle \Phi_b | V_f | \Psi_a^{(+)} \rangle = \langle \Phi_b | V_{pC} + V_{nC} | \Psi_a^{(+)} \rangle \quad (21.60a)$$

or

$$T_{ba}^d = \langle \Psi_b^{(-)} | V_i | \Phi_a \rangle = \langle \Psi_b^{(-)} | V_{pC} + V_{pN} | \Phi_a \rangle \quad (21.60b)$$

where [see eqs. (14.66)]

$$\Psi_a^{(+)} = \Phi_a + \frac{1}{E - H + i\varepsilon} V_i \Phi_a \quad (21.61a)$$

and

$$\Psi_b^{(-)} = \Phi_b + \frac{1}{E - H - i\varepsilon} V_f \Phi_b \quad (21.61b)$$

are unsymmetrized scattering wave functions and  $E = E_a = E_b$ .

We may use the methods of Section 16.6 to carry out the antisymmetrization of the scattering matrix with respect to the proton and neutron coordinates. The interchange of the incident proton with the  $i$ th proton in the target leads to the exchange transition matrix element

$$T_{ba}^{ex} = \langle \Phi_{b(i)} | V_{pC} + V_{nC} | \Psi_a^{(+)} \rangle \quad (21.62a)$$

where  $\Phi_{b(i)}$  corresponds to a new final state in which the incident proton has taken the place of the  $i$ th proton in the core. Similarly, we also have from eq. (21.60b)

$$T_{ba}^{ex} = \langle \Psi_b^{(-)} | V_{pC} + V_{pN} | \Phi_{a(i)} \rangle \quad (21.62b)$$

where  $\Phi_{a(i)}$  is a new initial state deduced from  $\Phi_a$  by interchanging the incident proton and the  $i$ th proton in the target. According to eq. (16.160), the transition matrix symmetrized in protons is then given by

$$\bar{T}_{ba}^{(p)} = T_{ba}^d - Z T_{ba}^{ex}. \quad (21.63)$$

The symmetrization with respect to the neutron coordinates may be done in a similar way. If  $T_{ba}^{(0)}$  is the transition matrix which singles out the optical neutron with coordinates  $r_0$  as the one to be found in the final deuteron, the transition matrix after neutron symmetrization is given by

$$\bar{T}_{ba}^{(n)} = \sqrt{N+1} T_{ba}^{(0)}. \quad (21.64)$$

Thus, collecting the results (21.63) and (21.64) we obtain for the transition matrix fully symmetrized in neutrons and protons

$$\bar{T}_{ba} = \sqrt{N+1} [T_{ba}^d - Z T_{ba}^{ex}]. \quad (21.65)$$

Further insight into the structure of eqs. (21.64)–(21.65) may be obtained if we use a *nuclear shell model* for the initial bound state wave function  $\psi_i$ . Let us display explicitly the neutron coordinates in the core wave function  $\psi_c(\xi)$  as

$$\psi_c(\xi) \equiv \psi_c(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N).$$

If we assume that the “optical” neutron is in a single orbital state  $\psi_n^{(i)}(\mathbf{r}_0, s_0)$  we may write

$$\psi_i = \frac{1}{\sqrt{N+1}} \left[ \psi_n^{(i)}(\mathbf{r}_0, s_0) \psi_c(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N) - \sum_{j=1}^N \psi_n^{(i)}(\mathbf{r}_j, s_j) \times \psi_c(\mathbf{r}_1, s_1, \dots, \mathbf{r}_{j-1}, s_{j-1}, \mathbf{r}_0, s_0, \mathbf{r}_{j+1}, s_{j+1}, \dots, \mathbf{r}_N, s_N) \right]. \quad (21.66)$$

Thus we see that if  $\psi_n^{(i)}$  is orthogonal to all the occupied states in  $\psi_c$ , and if the core remains inert, only the first term in eq. (21.66) will contribute to  $T_{ba}^{(0)}$ . Then, because of the factor  $(N+1)^{-1/2}$  in eq. (21.66), we find from eq. (21.64) that  $\bar{T}_{ba}^{(n)} = T_{ba}^{(0)}$  in this case. Since in this model the core is completely inert during the reaction it is also consistent to neglect the exchange contributions  $T_{ba}^{\text{ex}}$  so that eq. (21.65) becomes simply

$$\bar{T}_{ba} \simeq T_{ba}^d. \quad (21.67)$$

This last result is of course not surprising, since it corresponds to a pure three-body model of the pick-up reaction (21.29), in which the proton, the neutron *and the inert core C* are “elementary” particles. In what follows we shall therefore neglect the exchange terms  $T_{ba}^{\text{ex}}$  and concentrate our attention on the direct transition matrix  $T_{ba}^d$ .

In order to evaluate  $T_{ba}^d$ , we return to eqs. (21.60) and use the two-potential formalism of Chapter 17. We introduce the wave function

$$\chi_a^{(+)} = \Phi_a + \frac{1}{E - H_i + i\epsilon} V_{pC} \chi_a^{(+)} \quad (21.68)$$

which describes the scattering of a free proton by the core C (so that the distorting potential  $U_i$  in the initial state is simply  $V_{pC}$ ). Thus, writing

$$V_i = U_i + W_i \quad (21.69)$$

with  $U_i = V_{pC}$  and  $W_i = V_{pn}$ , we may use the Gell-Mann and Goldberger two-potential formula (17.42) together with the expression (21.58) of  $V_f$  to write the direct transition matrix as

$$T_{ba}^d = \langle \Phi_b | V_{pC} + V_{nC} - V_{pn} | \chi_a^{(+)} \rangle + \langle \Psi_b^{(-)} | V_{pn} | \chi_a^{(+)} \rangle. \quad (21.70)$$

The first matrix element on the right-hand side of this equation is easily seen to vanish. Indeed we first have

$$V_f \Phi_b = (V_{pC} + V_{nC}) \Phi_b = (H - H_f) \Phi_b = (H - E) \Phi_b$$

and since  $H = H_i + V_i$ , we may also write

$$(V_{pC} + V_{nC}) \Phi_b = (H_i + V_i - E) \Phi_b = (H_i + V_{pC} + V_{pn} - E) \Phi_b.$$

Hence the first term on the right-hand side of eq. (21.70) becomes

$$\langle \Phi_b | V_{pC} + V_{nC} - V_{pn} | \chi_a^{(+)} \rangle = \langle \Phi_b | H_i + V_{pC} - E | \chi_a^{(+)} \rangle. \quad (21.71)$$

However, from eq. (21.68) and the fact that  $(H_i - E)\Phi_a = 0$ , we deduce that

$$(H_i + V_{pC} - E - i\varepsilon) \chi_a^{(+)} = -i\varepsilon \Phi_a \quad (21.72)$$

and since  $\langle \Phi_b | \chi_a^{(+)} \rangle$  and  $\langle \Phi_b | \Phi_a \rangle$  are non singular [19], we see from eqs. (21.71) and (21.72) that in the limit  $\varepsilon \rightarrow 0^+$  we have

$$\langle \Phi_b | V_{pC} + V_{nC} - V_{pn} | \chi_a^{(+)} \rangle = 0. \quad (21.73)$$

We may therefore write the direct transition matrix for the pick-up process (21.29) as

$$T_{ba}^d = \langle \Psi_b^{(-)} | V_{pn} | \chi_a^{(+)} \rangle \quad (21.74)$$

With the choice (21.68) for the wave function  $\chi_a^{(+)}$  – corresponding to a distorting potential  $U_i = V_{pC}$  – the expression (21.74) of  $T_{ba}^d$  is still exact. However, the objects  $\chi_a^{(+)}$  and  $\Psi_b^{(-)}$  are many-body wave functions which are very difficult to obtain. For this reason we now discuss various approximation treatments whose starting point is the exact formula (21.74).

In order to orient ourselves here, we need some reasonable model of the pick-up reaction mechanism. According to the *direct nuclear reaction* model, the transition from the initial channel to the final channel in a nuclear reaction proceeds in *one step* without the formation of an intermediate state. This is in contrast with the *compound nucleus* model of nuclear reactions, in which the target nucleus first captures the incident particle to form a long lived compound nucleus: this compound nucleus subsequently decays to yield the various reaction products. In what follows we shall adopt the direct reaction model, which seems to be particularly suitable to describe nuclear reactions such as pick-up, stripping or knock-out (exchange) processes at intermediate and high energies. Thus, in the case of the pick-up reaction considered here, we expect the proton to pass near (or within) the target nucleus, and *suddenly* pick-up a neutron in order to form a deuteron. Thus, very little momentum will be transferred to the proton, and we expect the angular distribution to be enhanced at small angles. Furthermore, if we want to avoid the appearance of compound nucleus states in our description of the collision process, it is natural to keep only in the wave functions  $\chi_a^{(+)}$  and  $\Psi_b^{(-)}$  that part which corresponds to *elastic scattering*. We therefore write in that approximation

$$T_{ba}^d \simeq \langle \Psi_{cb}^{(-)} | V_{pn} | \chi_{ca}^{(+)} \rangle \quad (21.75)$$

where  $\chi_{ca}^{(+)}$  and  $\Psi_{cb}^{(-)}$  are respectively the elastic scattering parts of  $\chi_a^{(+)}$  and  $\Psi_b^{(-)}$ . According to the optical potential theory of Chapter 20, we find that

$$\chi_{ca}^{(+)} = \Phi_a + \frac{1}{E - H_i - \mathcal{V}_{\text{opt},i} + i\varepsilon} \mathcal{V}_{\text{opt},i} \Phi_a \quad (21.76)$$

where  $\mathcal{V}_{\text{opt},i}$  is the optical potential describing the elastic scattering of the proton by the core in the initial channel. Similarly we have

$$\Psi_{cb}^{(-)} = \Phi_b + \frac{1}{E - H_f - \mathcal{V}_{\text{opt},f} - i\varepsilon} \mathcal{V}_{\text{opt},f} \Phi_b \quad (21.77)$$

where  $\mathcal{V}_{\text{opt},f}$  is the optical potential which describes the elastic scattering of the deuteron by the core in the final channel. We note the strong similarity between eq. (21.75) and the DWBA matrix element (17.54). However, in the usual formulation of the DWBA method the distorting potential  $U_i^{\text{DW}}$  is chosen slightly differently: it is the optical potential describing the elastic scattering of the incident proton by the *target nucleus* X. If we call  $\chi_a^{(+)}$  the corresponding distorted wave such that

$$(H_i + U_i^{\text{DW}})\chi_a^{(+)} = E_a\chi_a^{(+)} \quad (21.78)$$

we may write the DWBA (direct) transition matrix element for the pick-up reaction (21.29) as [20]

$$T_{ba}^{\text{DWBA}} = \langle \Psi_{cb}^{(-)} | V_{pc} + V_{pn} - U_i^{\text{DW}} | \chi_a^{(+)} \rangle. \quad (21.79)$$

Returning now to eqs. (21.75)–(21.77), we recall that the optical potentials  $\mathcal{V}_{\text{opt},i}$  and  $\mathcal{V}_{\text{opt},f}$  are diagonal in the deuteron and nuclear internal states.

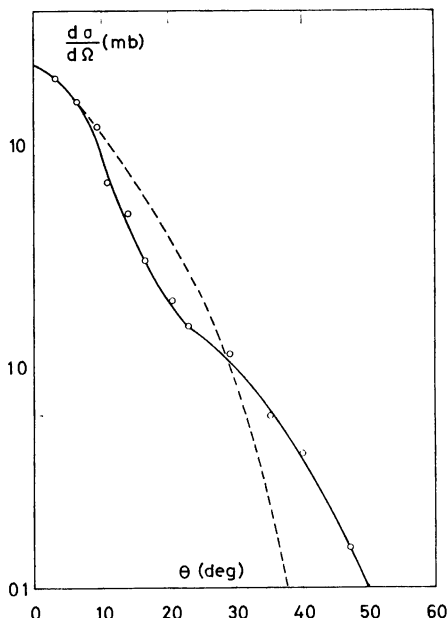


Fig. 21.4. The center of mass differential cross section for the pick-up reaction  $p + {}^{12}\text{C} \rightarrow d + {}^{11}\text{C}$  at an incident proton energy of 145 MeV. *Solid curve*: Optical model calculations of ref. [23] using eq. (21.75) and the eikonal approximation; *Dashed curve*: Plane wave calculations using eq. (21.98). The dots are the experimental points.



Thus, by writing [21]

$$\chi_{ca}^{(+)} = \sum_{\mathbf{v}_x} \psi_{i, \mathbf{v}_x} \phi_{k_i, \mathbf{v}_p, \mathbf{v}_x}^{(+)} \quad (21.80)$$

and

$$\Psi_{cb}^{(-)} = \sum_{\mathbf{v}_c} \psi_{t, \mathbf{v}_c} \phi_{k_t, \mathbf{v}_d, \mathbf{v}_c}^{(-)} \quad (21.81)$$

we may follow the method of Section 20.1 [see eqs. (20.42)–(20.46)] to obtain for  $\phi_{k_i, \mathbf{v}_p, \mathbf{v}_x}^{(+)}$  and  $\phi_{k_t, \mathbf{v}_d, \mathbf{v}_c}^{(-)}$  “potential scattering” equations involving the potentials  $\mathcal{V}_{\text{opt}, i}$  and  $\mathcal{V}_{\text{opt}, f}$ . Hence the wave functions  $\chi_{ca}^{(+)}$  and  $\Psi_{cb}^{(-)}$  and therefore the approximate expression (21.75) of the transition matrix, may be readily evaluated when a model has been chosen for the nuclear wave functions  $\psi_c$  and  $\psi_i$ , the deuteron wave function [22]  $\psi_d$  and the optical potentials  $\mathcal{V}_{\text{opt}, i}$  and  $\mathcal{V}_{\text{opt}, f}$ . We note that when the eikonal approximation may be used the functions  $\phi_{k_i, \mathbf{v}_p, \mathbf{v}_x}^{(+)}$  and  $\phi_{k_t, \mathbf{v}_d, \mathbf{v}_c}^{(-)}$  have the particularly simple form given by eq. (20.62). Such eikonal calculations have been performed by Greider [23]. We show in Fig. 21.4 a typical angular distribution obtained in this way (solid curve) for the reaction



at an incident proton energy of 145 MeV.

An even simpler approximation to the direct transition matrix element (21.74) may be obtained if we first write eq. (21.75) and then keep only the first term on the right-hand side of eqs. (21.76) and (21.77). That is,

$$\chi_{ca}^{(+)} \simeq \Phi_a, \quad \Psi_{cb}^{(-)} \simeq \Phi_b. \quad (21.83)$$

In this case we obtain the *plane wave approximation* to  $T_{ba}^d$ , namely

$$T_{ba}^{\text{PW}} = \langle \Phi_b | V_{pn} | \Phi_a \rangle \quad (21.84)$$

which we expect to be valid at sufficiently high energies, so that distortion of the incident and outgoing waves may be neglected. We note that the expression (21.84) differs from the first Born approximation to the matrix element (21.60b), namely

$$T_{ba}^d(\text{Born}) = \langle \Phi_b | V_{pc} + V_{pn} | \Phi_a \rangle. \quad (21.85)$$

By comparing eqs. (21.84) and (21.85) with the multiple scattering expansion (19.92) for a pick-up process (here  $V^3 \equiv V_{pn}$ ,  $T_2 \equiv T_{pc}$ , etc.) we see that the plane wave approximation (21.84) yields the first term in the multiple scattering expansion, while the first Born approximation also attempts to reproduce the second term by assuming that  $T_{pc} \simeq V_{pc}$ .

Let us now evaluate the expression (21.84). We shall neglect the D-wave component of the deuteron, thus assuming that the deuteron wave function  $\psi_d(\mathbf{r}_d, s_d)$  is a pure  ${}^3\text{S}_1$  state. Hence we write

$$\psi_d(\mathbf{r}_d, s_d) = \varphi_d(r_d) \chi_{1, v_d} \quad (21.86)$$

where the spatial part  $\varphi_d$  of the deuteron wave function is now a pure S-wave.

We then use eqs. (21.41) and (21.53) to write eq. (21.84) as

$$T_{ba}^{PW} = (2\pi)^{-3} \langle \exp(i\mathbf{k}_f \cdot \mathbf{r}_f) \psi_C(\xi) \varphi_d(r_d) \chi_{1,v_d} | V_{pn} | \exp(i\mathbf{k}_i \cdot \mathbf{r}_i) \psi_i(\xi, \mathbf{r}_0, s_0) \chi_{1/2,v_p} \rangle \quad (21.87)$$

or

$$T_{ba}^{PW} = (2\pi)^{-3} \int d\xi d\mathbf{r}_0 d\mathbf{r}_d \exp[-i\mathbf{k}_f \cdot (\mathbf{r}_0 - \frac{1}{2}\mathbf{r}_d)] \psi_C^\dagger(\xi) \varphi_d^*(r_d) \\ \times \chi_{1,v_d}^\dagger V_{pn}(\mathbf{r}_d) \exp\left[i\mathbf{k}_i \cdot \left(\frac{M_C}{M + M_C} \mathbf{r}_0 - \mathbf{r}_d\right)\right] \psi_i(\xi, \mathbf{r}_0, s_0) \chi_{1/2,v_p} \quad (21.88)$$

where a matrix product in spin space is understood and we have used Fig. 21.3 to deduce that

$$\mathbf{r}_i = \frac{M_C}{M + M_C} \mathbf{r}_0 - \mathbf{r}_d \quad (21.89a)$$

and

$$\mathbf{r}_f = \mathbf{r}_0 - \frac{1}{2}\mathbf{r}_d. \quad (21.89b)$$

We may also introduce the auxiliary vectors

$$\mathbf{K}_1 = \mathbf{k}_i - \frac{1}{2}\mathbf{k}_f \quad (21.90a)$$

and

$$\mathbf{K}_2 = \frac{M_C}{M + M_C} \mathbf{k}_i - \mathbf{k}_f \quad (21.90b)$$

so that eq. (21.88) becomes

$$T_{ba}^{PW} = (2\pi)^{-3} \int d\xi d\mathbf{r}_0 d\mathbf{r}_d \exp(-i\mathbf{K}_1 \cdot \mathbf{r}_d) \psi_C^\dagger(\xi) \varphi_d^*(r_d) \chi_{1,v_d}^\dagger \\ \times V_{pn}(\mathbf{r}_d) \exp(i\mathbf{K}_2 \cdot \mathbf{r}_0) \psi_i(\xi, \mathbf{r}_0, s_0) \chi_{1/2,v_p}. \quad (21.91)$$

Next, we eliminate the potential  $V_{pn}$  by using the Schrödinger equation for  $\varphi_d$ . Thus

$$V_{pn} \varphi_d(r_d) = \left( w_d + \frac{\hbar^2}{M} \nabla_{r_d}^2 \right) \varphi_d(r_d) \quad (21.92)$$

and we have

$$T_{ba}^{PW} = (2\pi)^{-3} \int d\mathbf{r}_d \exp(-i\mathbf{K}_1 \cdot \mathbf{r}_d) \left[ w_d + \frac{\hbar^2}{M} \nabla_{r_d}^2 \right] \varphi_d^*(r_d) \chi_{1,v_d}^\dagger \\ \times \int d\xi d\mathbf{r}_0 \psi_C^\dagger(\xi) \exp(i\mathbf{K}_2 \cdot \mathbf{r}_0) \psi_i(\xi, \mathbf{r}_0, s_0) \chi_{1/2,v_p}. \quad (21.93)$$

Introducing the Fourier transform  $\tilde{\varphi}_d(\mathbf{q})$  of the deuteron spatial wave function, namely

$$\tilde{\varphi}_d(\mathbf{q}) = (2\pi)^{-3/2} \int d\mathbf{r}_d \exp(i\mathbf{q} \cdot \mathbf{r}_d) \varphi_d(r_d) \quad (21.94)$$

we may write eq. (21.93) as

$$T_{ba}^{PW} = -(2\pi)^{-3/2} \left[ |w_d| + \frac{\hbar^2}{M} K_1^2 \right] \tilde{\phi}_d^*(K_1) \chi_{1,va}^\dagger \int d\xi d\mathbf{r}_0 \psi_c^\dagger(\xi) \\ \times \exp(i\mathbf{K}_2 \cdot \mathbf{r}_0) \psi_i(\xi, \mathbf{r}_0, s_0) \chi_{1/2, v_p}. \quad (21.95)$$

We may now perform the integrals on the variables  $\xi$  and  $\mathbf{r}_0$  by choosing the shell model form (21.66) of the wave function  $\psi_i$ . We assume again that  $\psi_n^{(i)}(\mathbf{r}_0, s_0)$  is orthogonal to the occupied states in  $\psi_c(\xi)$  and we find that the transition matrix (symmetrized in neutrons) is given by

$$\bar{T}_{ba}^{(n)} = - \left[ |w_d| + \frac{\hbar^2}{M} K_1^2 \right] \tilde{\phi}_d^*(K_1) \langle \chi_{1,va} | \tilde{\psi}_n^{(i)}(\mathbf{K}_2, s_0) \chi_{1/2, v_p} \rangle. \quad (21.96)$$

Here we have used the fact that

$$(2\pi)^{-3/2} \int d\xi d\mathbf{r}_0 \exp(i\mathbf{K}_2 \cdot \mathbf{r}_0) \psi_c^\dagger(\xi) \psi_c(\xi) \psi_n^{(i)}(\mathbf{r}_0, s_0) \\ = (2\pi)^{-3/2} \int d\mathbf{r}_0 \exp(i\mathbf{K}_2 \cdot \mathbf{r}_0) \psi_n^{(i)}(\mathbf{r}_0, s_0) = \tilde{\psi}_n^{(i)}(\mathbf{K}_2, s_0)$$

where  $\tilde{\psi}_n^{(i)}$  is the Fourier transform of  $\psi_n^{(i)}$ .

The differential cross section for the pick-up reaction, arising from the plane wave approximation (21.84), and neglecting the proton exchange terms, is then given by

$$\frac{d\bar{\sigma}}{d\Omega} = (2\pi)^4 \frac{M_i M_f}{\hbar^4} \frac{k_f}{k_i} \frac{1}{4} \sum_{v_p, v_d, v_n} |\bar{T}_{ba}^{(n)}|^2_{av} \quad (21.97)$$

where  $M_i$  and  $M_f$  are given respectively by eqs. (21.33) and (21.46). In obtaining the result (21.97) we have averaged over the initial spin orientations of the optical neutron [24] and summed over the final spin orientations of the deuteron [25]. Furthermore, the subscript *av* implies an average over the orientations of the optical neutron orbital angular momentum. Hence, using eq. (21.96), we find that

$$\frac{d\bar{\sigma}}{d\Omega} = (2\pi)^4 \frac{M_i M_f}{\hbar^4} \frac{k_f}{k_i} \left[ |w_d| + \frac{\hbar^2}{M} (\mathbf{k}_i - \frac{1}{2}\mathbf{k}_f)^2 \right]^2 |\tilde{\phi}_d(|\mathbf{k}_i - \frac{1}{2}\mathbf{k}_f|)|^2 \\ \times \frac{1}{4} \sum_{v_p, v_d, v_n} \left| \left\langle \chi_{1,va} \left| \tilde{\psi}_n^{(i)} \left( \frac{M_c}{M + M_c} \mathbf{k}_i - \mathbf{k}_f, s_0 \right) \chi_{1/2, v_p} \right\rangle \right|_{av}^2 \quad (21.98)$$

which is essentially the result obtained by Chew and Goldberger [26]. A comparison of the results arising from the simple formula (21.98) with those of the eikonal optical model of Greider – based on eq. (21.75) – is given in Fig. 21.4. It may be seen that the optical model calculation, which takes into account the strong absorption of the incident protons and the outgoing deuterons in the nucleus yields a larger number of deuterons at large scattering angles.

Since the pick-up and stripping reactions are related by time reversal, the differential cross section for the *stripping* reaction (21.27) may be obtained

from the corresponding pick-up cross section by applying the principle of detailed balance (see Section 16.7).

We shall not give here a detailed account of pick-up and stripping reactions at lower energies [27]. We simply note that these processes yield angular distributions which depend strongly on the orbital angular momentum of the “optical” nucleon. They provide therefore an important tool in nuclear spectroscopy.

## 21.3. Final state interactions

### 21.3.1. Introduction

We shall now consider a class of problems for which it is physically meaningful to separate the interactions acting during the collision into

i) a *primary interaction* which may be considered as responsible for the process under investigation (i.e. without which the transition would not occur) and

ii) *initial* and (or) *final state interactions* describing other interactions among the particles in the initial and final channels.

The basic contributions to final state interaction theory are those of Fermi [28] and Watson [29].

As an example, consider the photoelectric effect in atoms,



In this process a photon incident on a neutral atom  $A$  ejects an atomic electron, leaving an ion  $A^+$  and a free electron in the final state. The primary interaction is clearly the photon–electron interaction, while the final state interaction is the Coulomb attraction between the electron and the ion  $A^+$ . As we shall see below, this Coulomb interaction has a profound influence on the spectrum of the photoelectrons.

The interest of separating the dynamics of the collision into a primary interaction and initial (final) state interactions is twofold. Firstly, if we want to investigate the nature of the primary interaction, it is important to eliminate as thoroughly as possible the effects of initial or (and) final state interactions, and therefore to know how to treat these interactions “exactly”. For example, in many nuclear reactions we want to eliminate the effects of the Coulomb interaction which acts as a distorting potential in the initial and (or) final states.

On the contrary, if we suppose that the primary interaction is known, we can try to determine the characteristic parameters of the initial or final state interactions. For example, we may obtain useful information about the pion–nucleon interaction by analyzing the influence of the final state interaction between the pion and the nucleon in the photomeson production reaction  $\gamma + N \rightarrow N + \pi$  (where  $\gamma$  denotes a  $\gamma$ -ray). Similarly, information about the nucleon–nucleon interaction may be extracted from the final state

interaction arising in the process  $\gamma + d \rightarrow n + p$ , or from the initial state interaction occurring in the reaction  $N + N \rightarrow d + \pi$ . Final state interactions also play an important role in production experiments, where they may be used to study the forces acting between particles on which direct experiments are difficult to perform. For example the production reaction  $\pi + N \rightarrow \pi + \pi + N$  may serve to investigate the properties of the pion-pion system through their interaction in the final state. Quite generally, final state interactions occurring in production experiments may yield very useful results about the properties of short lived "elementary particles" (resonances) which are produced during the "primary interaction" step of the collision.

In what follows we shall only treat some simple aspects of final (initial) state interactions. Although the methods of dispersion theory may be applied to final state interaction problems [30] we shall confine ourselves to the case of interactions which may be described by potentials. Hence, the *two-potential formalism* developed in Chapter 17 may be directly applied.

To see how this may be done, let us first consider the simple case where the initial and final channels contain no bound states, so that there is only one arrangement channel. Let us call  $V$  the full interaction between the particles, and assume that we may separate it as  $V = U + W$ . Here  $W$  is the *primary interaction* responsible for the transition (i.e. such that if  $W = 0$  the process does not occur) while the remaining potential  $U$  is responsible for *initial* or *final state interactions*. For example, in the production process



the primary interaction  $W$  represents a phenomenological potential for pion production, while  $U$  describes the force acting between the two nucleons. Thus  $U$  is a phenomenological nucleon-nucleon potential, taking into account the effect of virtual mesons, but we assume that it cannot create real mesons.

Let us recall the two-potential formulae (17.44)–(17.45) appropriate for this case [31]. The transition matrix on the energy shell is given by

$$\langle b | \mathcal{T} | a \rangle = \langle \chi_b^{(-)} | U | \Phi_a \rangle + \langle \chi_b^{(-)} | W | \Psi_a^{(+)} \rangle \quad (21.101a)$$

or

$$\langle b | \mathcal{T} | a \rangle = \langle \Phi_b | U | \chi_a^{(+)} \rangle + \langle \Psi_b^{(-)} | W | \chi_a^{(+)} \rangle. \quad (21.101b)$$

Here  $\Phi_a$  and  $\Phi_b$  are the initial and final free states such that

$$\begin{aligned} H_0 \Phi_a &= E_a \Phi_a \\ H_0 \Phi_b &= E_b \Phi_b; \quad E_a = E_b = E \end{aligned} \quad (21.102)$$

where the unperturbed Hamiltonian  $H_0$  is simply the sum of the kinetic energies of the particles. The complete wave functions are given by

$$\begin{aligned} \Psi_a^{(+)} &= \Phi_a + \frac{1}{E - H_0 - U - W + i\varepsilon} (U + W) \Phi_a \\ &= \chi_a^{(+)} + \frac{1}{E - H_0 - U - W + i\varepsilon} W \chi_a^{(+)} \end{aligned} \quad (21.103a)$$

and

$$\begin{aligned}\Psi_b^{(-)} &= \Phi_b + \frac{1}{E - H_0 - U - W - i\varepsilon}(U + W)\Phi_b \\ &= \chi_b^{(-)} + \frac{1}{E - H_0 - U - W - i\varepsilon}W\chi_b^{(-)}\end{aligned}\quad (21.103b)$$

while the waves  $\chi_a^{(+)}$  and  $\chi_b^{(-)}$  are such that

$$\chi_a^{(+)} = \Phi_a + \frac{1}{E - H_0 - U + i\varepsilon}U\Phi_a \quad (21.104a)$$

and

$$\chi_b^{(-)} = \Phi_b + \frac{1}{E - H_0 - U - i\varepsilon}U\Phi_b. \quad (21.104b)$$

Now the wave functions  $\Phi_b$  and  $\chi_b^{(-)}$  contain a meson, while  $\Phi_a$  and  $\chi_a^{(+)}$  do not. Since the potential  $U$  cannot create mesons, we see that the first term on the right-hand side of eqs. (21.101) vanishes and the transition matrix element is given by

$$\langle b|\mathcal{T}|a\rangle = \langle \chi_b^{(-)}|W|\Psi_a^{(+)}\rangle \quad (21.105a)$$

or

$$\langle b|\mathcal{T}|a\rangle = \langle \Psi_b^{(-)}|W|\chi_a^{(+)}\rangle. \quad (21.105b)$$

If we write approximately  $\Psi_a^{(+)} \simeq \chi_a^{(+)}$  and  $\Psi_b^{(-)} \simeq \chi_b^{(-)}$  and substitute these expressions in eqs. (21.105) we obtain the simple formula

$$\langle b|\mathcal{T}|a\rangle \simeq \langle \chi_b^{(-)}|W|\chi_a^{(+)}\rangle \quad (21.106)$$

valid to first order in the primary interaction  $W$ , and to “all orders” in  $U$ .

When bound states are present the discussion becomes more involved. We may use the more general two potential formulae (17.41)–(17.42) to write the transition matrix as

$$\langle b|\mathcal{T}|a\rangle = \langle \chi_b^{(-)}|V_i - W_f|\Phi_a\rangle + \langle \chi_b^{(-)}|W_f|\Psi_a^{(+)}\rangle \quad (21.107a)$$

or

$$\langle b|\mathcal{T}|a\rangle = \langle \Phi_b|V_f - W_i|\chi_a^{(+)}\rangle + \langle \Psi_b^{(-)}|W_i|\chi_a^{(+)}\rangle \quad (21.107b)$$

where the objects  $\Phi_a$ ,  $\chi_a^{(+)}$ ,  $\Psi_a^{(+)}$ ,  $\Phi_b$ ,  $\chi_b^{(-)}$ ,  $\Psi_b^{(-)}$  are defined in Section 17.1 and we recall that the complete Hamiltonian  $H$  is decomposed in the initial arrangement channel as

$$H = H_i + V_i = H_i + U_i + W_i \quad (21.108a)$$

and in the final arrangement channel as

$$H = H_f + V_f = H_f + U_f + W_f. \quad (21.108b)$$

If the potentials  $U_i$  and  $U_f$  cannot produce the transition considered, eqs. (21.107) reduce to

$$\langle b|\mathcal{T}|a\rangle = \langle \chi_b^{(-)}|W_f|\Psi_a^{(+)}\rangle \quad (21.109a)$$

or

$$\langle b|\mathcal{T}|a\rangle = \langle \Psi_b^{(-)}|W_i|\chi_a^{(+)}\rangle. \quad (21.109b)$$

Moreover, let us choose the distorting potentials  $U_i$  and  $U_f$  as the optical potentials which generate the elastic scattering of the particles involved respectively in the initial and final channels. If we replace in eqs. (21.109) the unknown total wave functions  $\Psi_a^{(+)}$  and  $\Psi_b^{(-)}$  respectively by the distorted waves  $\chi_a^{(+)}$  and  $\chi_b^{(-)}$  corresponding to the scattering by the potentials  $U_i$  and  $U_f$  we obtain the DWBA transition matrix element

$$\langle b|\mathcal{T}|a\rangle_{\text{DWBA}} = \langle \chi_b^{(-)}|W_f|\chi_a^{(+)}\rangle = \langle \chi_b^{(-)}|W_i|\chi_a^{(+)}\rangle \quad (21.110)$$

valid to first order in the primary interactions  $W_i$  or  $W_f$ , and to “all orders” in  $U_i$  and  $U_f$ .

An interesting example of the application of two-potential formulae to a process in which initial and final states contain bound states is the pick-up reaction which we have already analyzed in Section 21.2. In this case we can use the DWBA expression (21.110) or alternatively recast the  $T$ -matrix element into the form [see eq. (21.74)]

$$\langle b|\mathcal{T}|a\rangle = \langle \Psi_b^{(-)}|V_{\text{pn}}|\chi_a^{(+)}\rangle \quad (21.111)$$

which explicitly displays the role of the primary interaction  $V_{\text{pn}}$  and incorporates the interaction  $V_{\text{pc}}$  into the functions  $\Psi_b^{(-)}$  and  $\chi_a^{(+)}$ .

### 21.3.2. Enhancement factors

Let us analyze more closely the matrix element (21.105a), namely [32]

$$\langle b|\mathcal{T}|a\rangle = \langle \chi_b^{(-)}|W|\Psi_a^{(+)}\rangle. \quad (21.112)$$

This expression plays a central role in final state interaction problems [33]. Since we expect that most of the final state effects are contained in  $\chi_b^{(-)}$  it is reasonable to compare the matrix element (21.112) with the expression

$$\langle b|\mathcal{T}^0|a\rangle = \langle \Phi_b|W|\Psi_a^{(+)}\rangle. \quad (21.113)$$

Suppose that the wave function  $\chi_b^{(-)}$  is the incoming scattering wave describing the motion of two final particles C and D interacting through a strongly attractive potential  $U$ . If we let the reaction proceed in the time-reversed sense, we expect that the presence of the interaction  $U$  would enhance the probability that the particles C and D remain together to enter the region of primary interaction. Then, using time reversal invariance [29] we see that the transition matrix (21.112) will be enhanced with respect to that of eq. (21.113) because of the interaction  $U$ . Let us write

$$\langle b|\mathcal{T}|a\rangle = \mathcal{F}\langle b|\mathcal{T}^0|a\rangle \quad (21.114)$$

where  $\mathcal{F}$  is a quantity to be determined. If we assume that the primary interaction  $W$  takes place over a very small region of space, and that we are sufficiently close to threshold so that only S-waves must be considered, we may write

$$\mathcal{F} = \frac{\mathcal{T}_s}{\mathcal{T}_s^0} \simeq \left[ \frac{\chi_0^{(-)*}(k, r)}{(2/\pi)^{1/2} j_0(k, r)} \right]_{r=0} \quad (21.115)$$

where  $\mathcal{T}_s$  and  $\mathcal{T}_s^0$  are respectively the S-wave parts of the matrix elements  $\langle b|\mathcal{T}|a\rangle$  and  $\langle b|\mathcal{T}^0|a\rangle$ . Moreover, we have written

$$\chi_b^{(-)}(\mathbf{k}, \mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \chi_l^{(-)}(k, r) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}),$$

and

$$\Phi_b(\mathbf{k}, \mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}) = (2/\pi)^{1/2} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}})$$

with

$$\chi_0^{(-)}(k, r) = (2/\pi)^{1/2} \exp\{-i\delta_0(k)\} \frac{u_0(k, r)}{kr}.$$

Here  $u_0(k, r)$  is the regular solution of the radial equation

$$\left[ \frac{d^2}{dr^2} + k^2 - U(r) \right] u_0(k, r) = 0$$

such that

$$u_0(k, r) \xrightarrow{r \rightarrow \infty} \sin(kr + \delta_0).$$

Hence

$$\tilde{\mathcal{F}} = \left[ \frac{\exp\{i\delta_0(k)\} u_0(k, r)}{\sin kr} \right]_{r=0} \quad (21.116)$$

and by comparison with eq. (11.82), [in which we choose  $A(k) = 1$ ] we see that

$$\tilde{\mathcal{F}} = \mathcal{F} \exp\{i\delta_0(k)\} = \frac{\exp\{i\delta_0(k)\}}{f(k)} \quad (21.117)$$

where  $f(k)$  is the Jost function introduced in Section 11.1. Using eq. (11.79) and the definition  $D(E) = f(-k)$  we also have

$$\tilde{\mathcal{F}} = \frac{1}{f(-k)} = \frac{1}{D(E)} \quad (21.118)$$

with  $D(E) = |D(E)| \exp\{-i\delta_0(E)\}$ , [see eq. (11.252)]. Hence, using eq. (21.115) and the above relations, we have

$$\mathcal{T}_s \simeq \frac{1}{D(E)} \mathcal{T}_s^0 \quad (21.119)$$

or

$$\mathcal{T}_s \simeq \frac{\exp\{i\delta_0(E)\}}{|D(E)|} \mathcal{T}_s^0. \quad (21.120)$$

We remark that the quantity  $\mathcal{T}_s^0$ , obtained by neglecting final state effects, represents a “first Born” value which is nearly energy independent because



of the short range of the primary interactions. Hence the energy dependence of  $\mathcal{T}_s$  is governed by the factor  $[D(E)]^{-1}$ . Moreover, we note that  $\mathcal{T}_s = |\mathcal{T}_s| \exp[i\delta_0(E)]$ , an important result to which we shall return below in connection with the Fermi–Watson theorem.

Returning to eq. (21.114) we see that the cross section obtained from the transition matrix element  $\langle b|\mathcal{T}|a\rangle$  is given by

$$\sigma_{ba} = |\mathcal{F}|^2 \sigma_{ba}^{(o)} \quad (21.121)$$

where  $\sigma_{ba}^{(o)}$  is the cross section corresponding to the transition matrix (21.113) and the *enhancement factor*  $|\mathcal{F}|^2 = |\mathcal{F}|^2$  measures the probability of finding the two particles (interacting through the potential  $U$ ) at the origin, relative to that when there is no interaction.

### 21.3.3. Unitarity and the Fermi–Watson theorem

Let us investigate the role played by the unitarity relations in initial and final state interactions. Starting from eq. (15.168a) and assuming time-reversal invariance (so that  $T_{ba} = T_{ab}$ ) we obtain

$$\text{Im } T_{ba} = -\pi \sum_n \delta(E_n - E) \delta(\mathbf{P}_n - \mathbf{P}_a) T_{bn} T_{an}^* \quad (21.122)$$

In what follows we shall focus our attention on two-body reactions of the type  $A + B \rightarrow C + D$ . We may then analyze eq. (21.122) in partial waves by following essentially the method used in Section 18.1. The result is

$$\begin{aligned} \text{Im } T_{ba}^l = & -\pi [T_{ba}^l T_{aa}^{l*} \rho_a \Theta(E - \bar{E}_a) + T_{bb}^l T_{ab}^{l*} \rho_b \Theta(E - \bar{E}_b) \\ & + \sum_{n \neq a, b} T_{bn}^l T_{an}^{l*} \rho_n \Theta(E - \bar{E}_n)] \end{aligned} \quad (21.123)$$

where we have isolated the contributions of the initial and final channels. Here the  $\rho$ 's are phase space factors (i.e. the density of states in the various channels),  $E = E_a = E_b$  is the total energy available in the C.M. system and  $\bar{E}_a, \bar{E}_b, \bar{E}_n$  are the energies necessary to reach the thresholds for the channels  $a, b, n$ . The function  $\Theta$  is the step function such that

$$\begin{aligned} \Theta(x) &= 1, \quad x > 0 \\ &= 0, \quad x < 0. \end{aligned} \quad (21.124)$$

Let us assume that we may neglect the “indirect” reactions which proceed from the initial channel  $a$  to the final channel  $b$  via an intermediate channel  $n$ . We then obtain the approximate equation [34]

$$\text{Im } T_{ba}^l = -\pi [T_{ba}^l T_{aa}^{l*} \rho_a \Theta(E - \bar{E}_a) + T_{bb}^l T_{ab}^{l*} \rho_b \Theta(E - \bar{E}_b)]. \quad (21.125)$$

In the presence of inelastic scattering the diagonal elements of  $T$  may be parametrized as [compare with eq. (18.36)]

$$T_{aa}^l = -\frac{1}{2i\pi\rho_a} [\exp(2i\delta_l^a) - 1], \quad (21.126a)$$

$$T_{bb}^l = -\frac{1}{2i\pi\rho_b} [\exp(2i\delta_l^b) - 1], \quad (21.126b)$$

where  $\delta_i^a$  and  $\delta_i^b$  are *complex* phase shifts. If we write

$$\delta_i^i = \text{Re } \delta_i^i + i \text{Im } \delta_i^i, \quad i = a, b \quad (21.127)$$

and define the “inelasticity factors”

$$\eta_i^i = \exp(-2 \text{Im } \delta_i^i) \quad (21.128)$$

we may also write eqs. (21.126) as

$$T_{aa}^i = -\frac{1}{2i\pi\rho_a} [\eta_i^a \exp(2i \text{Re } \delta_i^a) - 1], \quad (21.129a)$$

$$T_{bb}^i = -\frac{1}{2i\pi\rho_b} [\eta_i^b \exp(2i \text{Re } \delta_i^b) - 1]. \quad (21.129b)$$

Substituting eqs. (21.129) into eq. (21.125), we deduce that

$$\begin{aligned} \text{Im } T_{ba}^i = & -\frac{1}{2i} [\eta_i^a \exp(-2i \text{Re } \delta_i^a) - 1] T_{ba}^i \\ & + \frac{1}{2i} [\eta_i^b \exp(2i \text{Re } \delta_i^b) - 1] T_{ba}^{i*}. \end{aligned}$$

Thus

$$\eta_i^a \exp(-2i \text{Re } \delta_i^a) T_{ba}^i = \eta_i^b \exp(2i \text{Re } \delta_i^b) T_{ba}^{i*}. \quad (21.130)$$

Let us write the complex numbers  $T_{ba}^i$  in the form

$$T_{ba}^i = |T_{ba}^i| e^{i\phi}. \quad (21.131)$$

Then eq. (21.130) becomes

$$\eta_i^a e^{2i\phi} = \eta_i^b \exp\{2i(\text{Re } \delta_i^a + \text{Re } \delta_i^b)\} \quad (21.132)$$

from which we deduce that

$$\eta_i^a = \eta_i^b \quad (21.133)$$

and [35]

$$\phi = \text{Re } \delta_i^a + \text{Re } \delta_i^b. \quad (21.134)$$

Hence, we conclude that the partial wave  $T$  matrix  $T_{ba}^i$  is given by

$$T_{ba}^i = |T_{ba}^i| \exp\{i(\text{Re } \delta_i^a + \text{Re } \delta_i^b)\}. \quad (21.135)$$

This remarkable relation, called the *Fermi–Watson theorem*, implies that the phase of the partial-wave transition matrix for a reaction  $A + B \rightarrow C + D$  is determined by the (real part of the) phase shifts for *elastic* scattering in the initial and final channels. We recall that the Fermi–Watson theorem is a direct consequence of the unitarity relations, time-reversal invariance and the neglect of “intermediate” channels in eq. (21.123).

Two important particular cases follow directly from eq. (21.135). If final state interactions dominate the scattering, we may write

$$T_{ba}^i \simeq |T_{ba}^i| \exp(i \text{Re } \delta_i^b). \quad (21.136)$$

This bears a strong resemblance to the result (21.120) which we derived above for S-wave scattering. Of course, if initial state interactions are predominant, we have

$$T_{ba}^I \simeq |T_{ba}^I| \exp(i \operatorname{Re} \delta_i^a). \quad (21.137)$$

As an application of the Fermi–Watson theorem, let us look at the reaction of photoproduction of pions from nucleons, namely

$$\gamma + N \rightarrow N + \pi \quad (21.138)$$

which we consider together with the elastic processes

$$\gamma + N \rightarrow \gamma + N \quad (21.139)$$

and

$$N + \pi \rightarrow N + \pi. \quad (21.140)$$

Thus the reaction of photoproduction (21.138) corresponds to the transition  $a \rightarrow b$ , while the Compton scattering on nucleons (21.139) corresponds to  $a \rightarrow a$  and pion–nucleon scattering (21.140) to  $b \rightarrow b$ . Because of the weakness of electromagnetic interactions with respect to strong interactions we see that the reaction (21.138) is an example of final state interactions. We may therefore apply the form (21.136) of the Fermi–Watson theorem to relate the phases of the photoproduction transition matrix elements to the phase shifts for pion–nucleon scattering. This result has been very useful in the analysis of the experimental data on the photoproduction of pions [36, 37].

#### 21.3.4. The photoelectric effect

As an illustration of the theory of final state interactions, we shall now analyze the photoelectric effect in atoms.

Consider a photon of energy  $E = h\nu = \hbar\omega$  incident on an atom which we assume to be in the ground state. If the photon is sufficiently energetic it may eject one or several electrons from the atom. This process of ionization by photon impact is called the *photoelectric effect* [38]. We shall consider here a particular (single) ionization process, in which the electron is ejected from an hydrogenic atom of atomic number  $Z$ .

Let  $\mathbf{r}$  be the coordinate of the electron,  $w_0$  the ground state energy of the hydrogenic atom and  $\psi_0(\mathbf{r})$  its ground state wave function. The atomic nucleus is considered here as a structureless object [39] of charge  $Ze$ . Furthermore, we assume its mass to be infinitely large with respect to that of the electron, so that we neglect the recoil motion of the nucleus. We also assume that the free electron in the final state is non-relativistic. Then, if  $\mathbf{k}_f$  denotes the wave vector of the ejected electron, its kinetic energy in the final state is  $\hbar^2 k_f^2 / 2m$ , where  $m$  is the electron mass. Conservation of energy then yields

$$\hbar\omega + w_0 = \hbar^2 k_f^2 / 2m \quad (21.141)$$

valid in the non-relativistic regime, for which

$$\hbar\omega \text{ (or } \hbar^2 k_f^2 / 2m) \ll mc^2. \quad (21.142)$$

Two interactions are clearly at work in the photoelectric effect: the *primary* interaction is the *photon-electron* interaction, responsible for the effect, while the *final state interaction* is the *Coulomb attraction* between the ejected electron and the residual ion.

Let us first neglect the final state interaction. We expect this approximation to be most reliable when the kinetic energy of the ejected electron is large, i.e. when

$$\hbar\omega \text{ (or } \hbar^2 k_f^2/2m) \gg |w_0| \quad (21.143)$$

and when the nuclear charge  $Ze$  is small. Moreover, we may take advantage of the smallness of the fine structure constant  $\alpha \simeq 1/137$  to treat the photon-electron coupling to first order. This calculation can be done by evaluating the first order  $S$  matrix element of quantum electrodynamics corresponding to photon absorption [40]. Another, less rigorous approach is to treat the interaction between the electron and the electromagnetic field in a semi-classical way [41], using first order time-dependent perturbation theory. The two methods lead to identical results in the case which we consider. The relevant transition matrix, *neglecting final state interactions*, is given by

$$\langle b|T^0|a\rangle = \frac{ie\hbar}{mc} \int d\mathbf{r} \Phi_b^*(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) \mathbf{A}_0 \cdot \nabla_r \psi_0(r) \quad (21.144)$$

where  $\mathbf{k}$  is the incident photon wave vector (with  $k = |\mathbf{k}| = \omega/c$ ) and

$$\Phi_b(\mathbf{r}) = (2\pi)^{-3/2} \exp(i\mathbf{k}_f \cdot \mathbf{r}) \quad (21.145)$$

is a plane wave describing the final state of the free electron in the absence of final state interactions. The external electromagnetic field is represented here by the vector potential

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_0 \exp\{i(\mathbf{k} \cdot \mathbf{r} - \omega t)\} + \mathbf{A}_0^* \exp\{-i(\mathbf{k} \cdot \mathbf{r} - \omega t)\}$$

where  $\mathbf{A}_0$  is a constant complex vector. The factor  $\exp(i\mathbf{k} \cdot \mathbf{r})$  is called the *retardation factor*. Because of the presence of the bound state wave function  $\psi_0(r)$  we see that when  $kd \ll 1$ , where  $d$  is a typical atomic length [42], we may set  $\exp(i\mathbf{k} \cdot \mathbf{r}) \simeq 1$  in eq. (21.144) so that

$$\langle b|T^0|a\rangle \simeq \frac{ie\hbar}{mc} \mathbf{A}_0 \cdot \int d\mathbf{r} \Phi_b^*(\mathbf{r}) \nabla_r \psi_0(r). \quad (21.146)$$

This is known as the *dipole approximation* to the matrix element (21.144). We shall return to this approximation below. For the moment, however, we analyze the more accurate expression (21.144). Assuming the radiation to be incident along the  $z$ -axis and polarized with its electric vector along the  $x$ -axis, we have

$$\langle b|T^0|a\rangle = (2\pi)^{-3/2} \frac{ie\hbar}{mc} A_0 \int d\mathbf{r} \exp(-i\mathbf{k}_f \cdot \mathbf{r}) \exp\left(i\frac{\omega}{c}z\right) \frac{\partial}{\partial x} \psi_0(r). \quad (21.147)$$

Integration by parts (or acting with the operator  $\partial/\partial_x$  on the left) then yields

$$\langle b|T^0|a\rangle = -(2\pi)^{-3/2} \frac{e\hbar A_0 k_{f,x}}{mc} \int d\mathbf{r} \psi_0(r) \exp(i\mathbf{K} \cdot \mathbf{r}) \quad (21.148)$$

where  $k_{f,x}$  is the component of the electron wave vector  $\mathbf{k}_f$  along the  $x$ -axis and

$$\mathbf{K} = \frac{\omega}{c} \hat{\mathbf{z}} - \mathbf{k}_f \quad (21.149)$$

is the wave vector transferred to the atom.

The incident photon flux  $F_i$  is obtained by dividing the incident intensity  $\omega^2 |A_0|^2 / 2\pi c$  by  $\hbar\omega$ . Thus

$$F_i = \frac{\omega}{2\pi\hbar} |A_0|^2. \quad (21.150)$$

The density of final states, corresponding to the normalization adopted in (21.145) is simply

$$\rho_b = mk_f / \hbar^2. \quad (21.151)$$

Hence the differential cross section  $d\sigma^0/d\Omega$  for the ejection of the electron by photons polarized along the  $x$ -axis (neglecting final state interactions) is given by

$$\frac{d\sigma^0}{d\Omega} = \frac{2\pi}{\hbar F_i} \rho_b |\langle b|T^0|a\rangle|^2$$

or

$$\frac{d\sigma^0(\theta, \phi)}{d\Omega} = \frac{e^2 k_f k_{f,x}^2}{2\pi m c \omega} \left| \int d\mathbf{r} \psi_0(r) \exp(i\mathbf{K} \cdot \mathbf{r}) \right|^2 \quad (21.152)$$

where  $(\theta, \phi)$  are the polar angles of the vector  $\mathbf{k}_f$ , so that  $k_{f,x} = k_f \sin \theta \cos \phi$ .

For an hydrogenic atom of nuclear charge  $Ze$  the ground state wave function  $\psi_0(r)$  is given by

$$\psi_0(r) = \frac{Z^{3/2}}{(\pi a_0^3)^{1/2}} \exp\left(-\frac{Zr}{a_0}\right), \quad a_0 = \frac{\hbar^2}{me^2} \quad (21.153)$$

so that

$$\frac{d\sigma^0(\theta, \phi)}{d\Omega} = \frac{32e^2 Z^5 a_0^3 k_f k_{f,x}^2}{mc\omega(Z^2 + K^2 a_0^2)^4}. \quad (21.154)$$

For an unpolarized photon beam an average must be made over the polarizations of the photon, so that  $k_{f,x}^2$  is replaced by  $\frac{1}{2}(k_{f,x}^2 + k_{f,y}^2)$ . The differential cross section becomes in this case

$$\frac{d\sigma^{(0)}(\theta)}{d\Omega} = \frac{16e^2 Z^5 a_0^3 k_f^3 \sin^2 \theta}{mc\omega(Z^2 + K^2 a_0^2)^4}. \quad (21.155)$$

We note that the factor  $\sin^2 \theta$  favours the ejection of electrons at right angles to the incident photon beam, while the presence of the quantity  $K$  in the denominator enhances the scattering at small angles since  $K$  is smallest in the forward direction. Now, at high incident photon energies such that the relation (21.143) is verified, we may neglect  $w_0$  in eq. (21.141) to infer that

$$\hbar^2 k_f^2 / 2m \simeq \hbar \omega \quad (21.156)$$

and therefore the velocity of the outgoing electron is simply

$$v_f = \hbar k_f / m \simeq 2\omega / k_f.$$

The quantity  $K^2$  is then given by

$$\begin{aligned} K^2 &= k_f^2 - 2\frac{\omega}{c} k_f \cos \theta + \frac{\omega^2}{c^2} \\ &= k_f^2 \left( 1 - \frac{v_f}{c} \cos \theta + \frac{v_f^2}{4c^2} \right) \simeq k_f^2 \left( 1 - \frac{v_f}{c} \cos \theta \right) \end{aligned}$$

where we have neglected terms of order  $(v_f/c)^2$  because the outgoing electron is non-relativistic. Moreover, since

$$w_0 = -\frac{e^2}{2a_0} Z^2 \quad (21.157)$$

for an hydrogenic atom, we deduce from the relations (21.143) and (21.157) that

$$k_f^2 a_0^2 \gg \frac{2m}{\hbar^2} |w_0| a_0^2 = Z^2.$$

Therefore the expression  $(Z^2 + K^2 a_0^2)$  which appears in the denominator of eq. (21.155) may be written approximately as

$$Z^2 + K^2 a_0^2 \simeq k_f^2 a_0^2 \left( 1 - \frac{v_f}{c} \cos \theta \right)$$

so that, dropping again terms of order  $(v_f/c)^2$ , we may write

$$(Z^2 + K^2 a_0^2)^{-4} = k_f^{-8} a_0^{-8} \left( 1 + \frac{4v_f}{c} \cos \theta \right). \quad (21.158)$$

Hence the factor  $(Z^2 + K^2 a_0^2)^{-4}$  influences the angular distribution only at rather high energies.

Returning to eq. (21.155), we have with the help of eq. (21.158)

$$\frac{d\sigma^{(o)}(\theta)}{d\Omega} = \frac{16e^2 Z^5}{mc\omega(k_f a_0)^5} \sin^2 \theta \left( 1 + \frac{4v_f}{c} \cos \theta \right) \quad (21.159)$$

or, by using eqs. (21.156) and (21.157)

$$\frac{d\sigma^{(o)}(\theta)}{d\Omega} = 32\alpha \frac{a_0^2}{Z^2} \left( \frac{|w_0|}{\hbar\omega} \right)^{7/2} \sin^2 \theta \left( 1 + \frac{4v_f}{c} \cos \theta \right), \quad (\alpha = e^2/\hbar c). \quad (21.160)$$

The total cross section at high energies, neglecting final state interactions, is then

$$\sigma_{\text{tot}}^{(o)} = \frac{256\pi}{3} \alpha \frac{a_o^2}{Z^2} \left( \frac{|w_0|}{\hbar\omega} \right)^{7/2} \quad (21.161)$$

and is proportional to  $(\hbar\omega)^{-7/2}$  and to  $Z^5$ . It is worth noting that the *dipole approximation* [obtained by setting  $\exp(i\omega z/c) = 1$  in eq. (21.147)] yields the *leading term* in the differential cross section (such that corrections of order  $v/c$  are neglected). Calling  $d\sigma_d^{(o)}/d\Omega$  this term, we have

$$\frac{d\sigma_d^{(o)}(\theta)}{d\Omega} = 32\alpha \frac{a_o^2}{Z^2} \left( \frac{|w_0|}{\hbar\omega} \right)^{7/2} \sin^2 \theta. \quad (21.162)$$

We also note that the dipole approximation yields the *complete* result (21.161) for the total cross section  $\sigma_{\text{tot}}^{(o)}$ .

We have obtained the total cross section  $\sigma_{\text{tot}}^{(o)}$  by using high-energy approximations in the expression (21.155) of the differential cross section and by integrating the resulting expression (21.160) over the angles. For further reference it is also interesting to integrate *directly* the differential cross section (21.155) over the angles. The result is

$$\hat{\sigma}_{\text{tot}}^{(o)} = \frac{256\pi}{3} \alpha \frac{a_o^2}{Z^2} \left( \frac{|w_0|}{\hbar\omega} \right)^5 \left\{ \frac{\hbar\omega - |w_0|}{|w_0|} \right\}^{3/2} \quad (21.163)$$

and represents therefore the total cross section which one obtains at *all* energies when final state interactions are neglected. Of course

$$\hat{\sigma}_{\text{tot}}^{(o)} \xrightarrow{\hbar\omega \gg |w_0|} \sigma_{\text{tot}}^{(o)} \quad (21.164)$$

but we note that  $\hat{\sigma}_{\text{tot}}^{(o)}$  vanishes at threshold, in contrast to  $\sigma_{\text{tot}}^{(o)}$ .

We now include final state interaction effects while treating always the primary electron-photon interaction to first order. To this end we simply replace in eq. (21.144) the plane wave  $\Phi_b$  by a distorted wave  $\chi_b^{(-)}$  which takes into account the Coulomb attraction between the electron and the ion. Thus  $\chi_b^{(-)}$  is a *Coulomb wave* which exhibits the asymptotic behaviour of a "plane" wave (with a distorted phase) plus an *incoming* spherical wave, and the transition matrix element, including final state interactions, is given by

$$\langle b|T|a \rangle = \frac{ie\hbar}{mc} \int d\mathbf{r} \chi_b^{(-)*}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) A_o \cdot \nabla_r \psi_o(\mathbf{r}). \quad (21.165)$$

If we are interested in the region of *low energies*, in particular near the *threshold* of the reaction (where we expect final state interactions to be important), we may use the *dipole approximation* and write  $\exp(i\mathbf{k} \cdot \mathbf{r}) \simeq 1$ . Then eq. (21.165) yields

$$\langle b|T|a \rangle \simeq \frac{ie\hbar}{mc} A_o \cdot \int d\mathbf{r} \chi_b^{(-)*}(\mathbf{r}) \nabla_r \psi_o(\mathbf{r}). \quad (21.166)$$

We recall that the dipole approximation is valid when

$$ka \ll 1, \quad a = a_0/Z$$

or [using eq. (21.157) and the fact that  $k = \omega/c$ ], when

$$\hbar\omega \ll |w_0|/Z\alpha, \quad \alpha \simeq 1/137 \quad (21.167)$$

so that its range of validity extends to the *intermediate energy region*.

We shall not carry out the detailed calculation of the matrix element (21.166). The result is [43]

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma_d^{(0)}}{d\Omega} C \quad (21.168)$$

where  $d\sigma_d^{(0)}/d\Omega$  is the dipole differential cross section (21.162) and

$$C = 2\pi \left[ \frac{|w_0|}{\hbar\omega} \right]^{1/2} \frac{\exp(-4n' \cot^{-1} n')}{1 - \exp(-2\pi n')} \quad (21.169)$$

with  $n' = Z/(k_f a_0)$ . We first note that for large values of  $k_f$  (i.e. small values of  $n'$ ) we may expand  $C$  about  $n' = 0$  and obtain

$$C \simeq [|w_0|/\hbar\omega]^{1/2}/n'.$$

However, by using eqs. (21.156) and (21.157), we have also

$$\frac{1}{n'} = \frac{k_f a_0}{Z} \simeq \frac{(2m)^{1/2}}{\hbar} (\hbar\omega)^{1/2} \frac{a_0}{Z} = \left[ \frac{\hbar\omega}{|w_0|} \right]^{1/2}$$

so that

$$\lim_{n' \rightarrow 0} C(n') = \lim_{k_f \rightarrow \infty} C(k_f) = 1 \quad (21.170)$$

and we verify (within the dipole approximation) that final state interactions are unimportant at high energies. It should be noted, however, that because of the infinite range of the Coulomb interaction the quantity  $C$  reaches its asymptotic value very slowly.

Let us now look at the behaviour of the cross section (21.168) near threshold. In this case we have

$$C = 2\pi \left[ \frac{|w_0|}{\hbar\omega} \right]^{1/2} e^{-4} \left( 1 + \frac{4}{3n'^2} \right), \quad (e = 2.71828). \quad (21.171)$$

But

$$\begin{aligned} \left\{ \frac{|w_0|}{\hbar\omega} \right\}^{1/2} &= \left\{ 1 - \frac{\hbar\omega - |w_0|}{\hbar\omega} \right\}^{1/2} \simeq \left\{ 1 - \frac{\hbar\omega - |w_0|}{|w_0|} \right\}^{1/2} \\ &\simeq 1 - \frac{1}{2} \frac{\hbar\omega - |w_0|}{|w_0|}. \end{aligned} \quad (21.172)$$

Moreover, from eqs. (21.141) and (21.157) we deduce that

$$\frac{1}{n'^2} = \frac{k_f^2 a_0^2}{Z^2} = \frac{2m}{\hbar^2} (\hbar\omega - |w_0|) \frac{a_0^2}{Z^2} = \frac{\hbar\omega - |w_0|}{|w_0|}$$



and therefore

$$1 + \frac{4}{3n'^2} = 1 + \frac{4}{3} \frac{\hbar\omega - |w_0|}{|w_0|}. \quad (21.173)$$

Hence, by substituting the expressions (21.172) and (21.173) into eq. (21.171), we find that

$$\begin{aligned} C &\simeq 2\pi e^{-4} \left\{ 1 - \frac{1}{2} \frac{\hbar\omega - |w_0|}{|w_0|} \right\} \left\{ 1 + \frac{4}{3} \frac{\hbar\omega - |w_0|}{|w_0|} \right\} \\ &\simeq 2\pi e^{-4} \left\{ 1 + \frac{5}{6} \frac{\hbar\omega - |w_0|}{|w_0|} + \dots \right\}. \end{aligned} \quad (21.174)$$

Using eqs. (21.162) and (21.168) we then obtain the differential cross section near threshold as

$$\frac{d\sigma(\theta)}{d\Omega} = 64\pi e^{-4} \alpha \frac{a_o^2}{Z^2} \sin^2 \theta \left\{ 1 - \frac{7}{2} \frac{\hbar\omega - |w_0|}{|w_0|} \right\} \left\{ 1 + \frac{5}{6} \frac{\hbar\omega - |w_0|}{|w_0|} \right\}$$

or

$$\frac{d\sigma(\theta)}{d\Omega} = 64\pi e^{-4} \alpha \frac{a_o^2}{Z^2} \sin^2 \theta \left\{ 1 - \frac{8}{3} \frac{\hbar\omega - |w_0|}{|w_0|} + \dots \right\}. \quad (21.175)$$

The total cross section  $\sigma_{\text{tot}}$ , including final state interactions, is obtained by integrating the expression (21.168) over the angles. This yields

$$\sigma_{\text{tot}} = \sigma_{\text{tot}}^{(0)} C \quad (21.176)$$

where  $\sigma_{\text{tot}}^{(0)}$  and  $C$  are given respectively by eqs. (21.161) and (21.169). Since we want to isolate final state effects over the whole range of (non-relativistic) energies, we must actually compare  $\sigma_{\text{tot}}$  to the cross section  $\hat{\sigma}_{\text{tot}}^{(0)}$  obtained in eq. (21.163). This gives

$$\sigma_{\text{tot}} = \hat{\sigma}_{\text{tot}}^{(0)} D \quad (21.177)$$

where

$$D = C \left\{ \frac{\hbar\omega}{\hbar\omega - |w_0|} \right\}^{3/2}. \quad (21.178)$$

The two cross sections  $\sigma_{\text{tot}}$  and  $\hat{\sigma}_{\text{tot}}^{(0)}$  are illustrated in Fig. 21.5 for the case of the photoelectric effect in atomic hydrogen. At high energies the quantity  $D$  approaches unity from below, so that  $\sigma_{\text{tot}}$  is *reduced* with respect to  $\hat{\sigma}_{\text{tot}}^{(0)}$  (or  $\sigma_{\text{tot}}^{(0)}$ ). On the contrary, at low energies the cross section  $\sigma_{\text{tot}}$  is enhanced with respect to  $\hat{\sigma}_{\text{tot}}^{(0)}$ . In particular by using eqs. (21.163), (21.174) and (21.178) we see that in contrast with  $\hat{\sigma}_{\text{tot}}^{(0)}$  which *vanishes* at threshold we find for  $\sigma_{\text{tot}}$  a *finite* threshold value

$$\sigma_{\text{tot}}(\text{thr}) = \frac{512\pi^2}{3} e^{-4} \alpha \frac{a_o^2}{Z^2}. \quad (21.179)$$

We note from Fig. 21.5 that  $\sigma_{\text{tot}}$  actually reaches its *maximum* value at threshold. This enhancement of the low-energy cross section is a striking illustration of final state interaction effects.

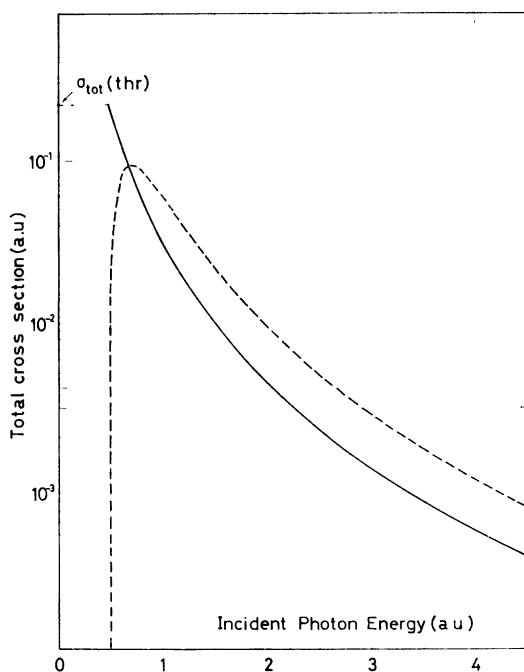


Fig. 21.5. The total cross section for the photoelectric effect in atomic hydrogen (in atomic units  $a_0^2$ ), as a function of the incident photon energy (in atomic units  $e^2/a_0$ ). *Dashed curve*: the quantity  $\hat{\sigma}_{\text{tot}}^{(0)}$  of the text (no final state interactions included); *Solid curve*: the quantity  $\sigma_{\text{tot}}$  (including final state interaction effects). The total cross section at threshold is  $\sigma_{\text{tot}}(\text{thr}) = 0.225 a_0^2$  [see eq. (21.179)].

## References and notes

- [1] We recall that atomic units (a.u.) are such that the unit of length is the Bohr radius  $a_0 = \hbar^2/me^2$  and the unit of energy is  $e^2/a_0$ , i.e. twice the Rydberg.
- [2] BYRON Jr., F. W. and C. J. JOACHAIN (1966), *Phys. Rev.* **146**, 1.
- [3] See Section 19.5, in particular the discussion following eq. (19.208).
- [4] BYRON Jr., F. W. and C. J. JOACHAIN (1973), *Phys. Rev.* **A8**, 1267.
- [5] BROMBERG, J. P. (1969), *J. Chem. Phys.* **50**, 3906.
- [6] BYRON Jr., F. W. and C. J. JOACHAIN (1973), *Phys. Rev.* **A8**, 3266.
- [7] We recall that at large momentum transfers the Born series is converging more slowly, so that the success of the EBS method depends delicately on cancellations between higher order terms. See ref. [6] and the discussion of the EBS method given in Section 19.5.
- [8] GERJUOY, E. and N. A. KRALL (1960), *Phys. Rev.* **119**, 705; (1962), *Phys. Rev.* **127**, 2105. Although this assumption is plausible, no proof of it has been given, the main difficulty being due to the presence of exchange effects.

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- [13] INOKUTI, M., Y. K. KIM and R. L. PLATZMAN (1967), *Phys. Rev.* **164**, 55.
- [14] It is worth noting, however, that this agreement is primarily a test of dispersion relations for the *direct* amplitude, since exchange effects are relatively small at the energies considered in Table 21.1.
- [15] It is also important to note that the target wave function  $\psi_i$  should only depend on the *A* relative coordinates of its (*A* + 1) constituent nucleons. Various methods are available to eliminate the coordinates of the C.M. of the target [see for example GARTENHAUS, S. and C. SCHWARTZ (1957), *Phys. Rev.* **108**, 482]. We shall assume that this operation has already been performed.
- [16] We shall assume that the core wave function  $\psi_c(\xi)$  has already been fully antisymmetrized with respect to the coordinates of its *Z* protons and *N* neutrons.
- [17] This state is such that the nucleons in the deuteron are considered to be distinct from those in the core C.
- [18] We neglect long range Coulomb forces between the deuteron and the core C.
- [19] We recall that the free waves  $\Phi_a$  and  $\Phi_b$  correspond to different arrangement channels.
- [20] A detailed analysis of the DWBA matrix element (21.79) may be found in TOBOCMAN, W. (1961), *Theory of Direct Nuclear Reactions* (Oxford Univ. Press).
- [21] In eqs. (21.80) and (21.81) the spin orientations of the proton, the target nucleus X, the core C and the deuteron are denoted respectively by  $\nu_p$ ,  $\nu_x$ ,  $\nu_c$  and  $\nu_d$ .
- [22] We recall that  $\psi_f = \psi_c \psi_d$  [see eq. (21.50)].
- [23] GREIDER, K. R. (1959), *Phys. Rev.* **114**, 786.
- [24] We denote by  $\nu_n$  the spin orientation of the optical neutron.
- [25] We have assumed for simplicity that the nuclear core C has spin zero. There is no difficulty, however, in generalizing eq. (21.97) to the case of a nuclear core of spin  $J_c$  and an initial nucleus X of total spin  $J_x$  (obtained by coupling the spin of the nuclear core to that of the optical neutron). See for example TOBOCMAN, W., *Theory of Direct Nuclear Reactions*, loc. cit. [20].
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- [31] GELL-MANN, M. and M. L. GOLDBERGER (1953), *Phys. Rev.* **91**, 398.
- [32] A similar analysis may evidently be carried out for the corresponding matrix element  $\langle \psi_b^{(-)} | W | \chi_a^{(+)} \rangle$ .
- [33] We follow here the treatment of ref. [29]. See also GOLDBERGER, M. L. and K. M. WATSON (1964), *Collision Theory* (Wiley, New York) Chapter 9.
- [34] This equation evidently becomes exact when only the initial and final channels are open.
- [35] We note that eq. (21.132) only determines  $\phi$  modulo  $\pi$ , since by changing  $\phi$  to  $\tilde{\phi} = \phi + \pi$  we leave eq. (21.132) invariant. Values of  $\tilde{\phi}$  differing from  $\phi$  modulo  $\frac{1}{2}\pi$  would lead to the result  $\eta_i^a = -\eta_i^b$  which is unphysical because  $\eta_i^a$  and  $\eta_i^b$  must be positive.

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- [37] WATSON, K. M., J. C. KECK, A. V. TOLLESTRUP and R. L. WALKER (1956), *Phys. Rev.* **101**, 1159.
- [38] The corresponding nuclear reaction, in which a nucleus is broken up by photon impact, is called *photodisintegration*.
- [39] This hypothesis evidently becomes invalid when the incident photon is highly energetic, in which case it can probe the internal structure of the nucleus.
- [40] See for example HEITLER, W. (1954), *The Quantum Theory of Radiation* (3rd ed., Oxford Univ. Press, New York).
- [41] See for example SCHIFF, L. I. (1955), *Quantum Mechanics* (second ed., McGraw-Hill, New York) Chapter 10.
- [42] For example we may take  $d \simeq a = a_0/Z$  where  $a_0 = \hbar^2/me^2$  is the first Bohr radius of the hydrogen atom.
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# Appendix A

## Principles of Quantum Mechanics

It is postulated in the usual formulation of quantum mechanics that all the information about a physical system at a given time can be derived from the knowledge of the *state vector* or *wave function*  $\Psi$  of the system. This wave function is a vector in *Hilbert space*, i.e. a linear vector space with an infinite number of dimensions and a metric [1]. Using Dirac's notation [2], we shall denote this vector by the ket  $|\Psi\rangle$ . The linear character of the space, which expresses the *superposition principle*, states that if  $|\Psi_1\rangle$  and  $|\Psi_2\rangle$  represent two possible physical states, while  $\alpha_1$  and  $\alpha_2$  are two arbitrary complex numbers, then the ket

$$|\Psi\rangle = \alpha_1|\Psi_1\rangle + \alpha_2|\Psi_2\rangle \quad (\text{A.1})$$

represents a new state vector in the same space.

The metric is introduced by defining a complex number, called the inner product or *scalar product* [3] of two vectors  $|\Psi_1\rangle$  and  $|\Psi_2\rangle$ , such that

$$\langle\Psi_1|\Psi_2\rangle = \langle\Psi_2|\Psi_1\rangle^*. \quad (\text{A.2a})$$

The object  $\langle\Psi|$  is called the conjugate bra of the ket  $|\Psi\rangle$ . If  $\alpha$  is a complex number and  $|\Psi_3\rangle$  a third vector, we also have

$$\langle\Psi_1|\alpha\Psi_2\rangle = \alpha\langle\Psi_1|\Psi_2\rangle, \quad (\text{A.2b})$$

$$\langle\alpha\Psi_1|\Psi_2\rangle = \alpha^*\langle\Psi_1|\Psi_2\rangle, \quad (\text{A.2c})$$

$$\langle\Psi_3|\Psi_1 + \Psi_2\rangle = \langle\Psi_3|\Psi_1\rangle + \langle\Psi_3|\Psi_2\rangle \quad (\text{A.2d})$$

where the asterisk denotes the complex conjugation.

The same physical state is represented by the vectors  $|\Psi\rangle$  or  $\alpha|\Psi\rangle$ , i.e. by a *ray* (or direction) in Hilbert space. It is customary to describe the state by a vector  $|\Psi\rangle$  normalized to one, i.e. such that

$$\langle\Psi|\Psi\rangle = 1. \quad (\text{A.3})$$

In this way only a constant phase factor (i.e. a multiplicative factor of modulus one) is left undetermined. It is worth noting that not all the rays of Hilbert space correspond to physical states. In fact, physically allowed rays must satisfy certain conditions which are called *superselection rules* [4]; these constraints arise from the requirement that certain physical quantities (such as the total electric charge) must keep definite and constant values for a closed physical system.

Before we proceed further with the principles of quantum mechanics, let us recall a few definitions concerning operators in (linear) vector spaces. Let  $|\Psi_1\rangle$  and  $|\Psi_2\rangle$  be two vectors in a given vector space, while  $\alpha_1$  and  $\alpha_2$  are complex numbers. An operator  $A$  is called *linear* if

$$A[\alpha_1|\Psi_1\rangle + \alpha_2|\Psi_2\rangle] = \alpha_1 A|\Psi_1\rangle + \alpha_2 A|\Psi_2\rangle \quad (\text{A.4})$$

and *antilinear* if

$$A[\alpha_1|\Psi_1\rangle + \alpha_2|\Psi_2\rangle] = \alpha_1^* A|\Psi_1\rangle + \alpha_2^* A|\Psi_2\rangle. \quad (\text{A.5})$$

A linear operator is *bounded* if there exists a positive number  $C$  such that

$$\|A\Psi\| \leq C\|\Psi\| \quad (\text{A.6})$$

where  $\|x\| = (\langle x|x \rangle)^{1/2}$  is called the *norm* of the vector  $|x\rangle$ .

Let us now consider a set  $|\chi_i\rangle$  of vectors of the space which are *orthonormal*, i.e.

$$\langle \chi_i | \chi_j \rangle = \delta_{ij} \quad \text{or} \quad \delta(i - j). \quad (\text{A.7})$$

In other words, these vectors are *orthogonal* and *normalized*. The object  $\delta_{ij}$  appearing in eq. (A.7) is called the Kronecker symbol. It is such that

$$\delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j. \end{cases} \quad (\text{A.8})$$

If the vectors are labelled by continuous indices, then we must use on the right-hand side of eq. (A.7) the Dirac  $\delta$ -function, such that

$$\int f(x) \delta(x - y) dx = f(y). \quad (\text{A.9})$$

We shall also assume that the set of vectors  $|\chi_i\rangle$  is *complete*, so that any vector  $|\Psi\rangle$  in the space may be expressed in terms of the vectors  $|\chi_i\rangle$  as

$$|\Psi\rangle = \sum_i c_i |\chi_i\rangle. \quad (\text{A.10})$$

The set  $\{\chi_i\}$  of vectors  $|\chi_i\rangle$  is then called a *basis* of the vector space. The complex coefficients  $c_i$  are the *components* of the vector  $|\Psi\rangle$  in the basis  $\{\chi_i\}$ . We note that once a given basis – also called a *representation* – has been chosen, a vector  $|\Psi\rangle$  is completely specified by its components  $c_i$ . Furthermore, we have

$$c_i = \langle \chi_i | \Psi \rangle. \quad (\text{A.11})$$

The action of an operator  $A$  on a given vector  $|\Psi\rangle$  may be specified in terms of its effect on the components  $c_i$  in a given representation. Indeed, starting from eq. (A.10), we have, for a linear operator  $A$ ,

$$A|\Psi\rangle = A \sum_i c_i |\chi_i\rangle = \sum_i c_i A|\chi_i\rangle. \quad (\text{A.12})$$

Let us express the new vectors  $|\chi'_i\rangle = A|\chi_i\rangle$  in our basis as

$$|\chi'_i\rangle = A|\chi_i\rangle = \sum_j A_{ji} |\chi_j\rangle \quad (\text{A.13})$$

where the complex numbers  $A_{ji}$  are given by

$$A_{ji} = \langle \chi_j | A | \chi_i \rangle. \quad (\text{A.14})$$

Then, if we write

$$|\Psi'\rangle = A|\Psi\rangle = \sum_j d_j |\chi_j\rangle \quad (\text{A.15})$$

so that the coefficients  $d_j$  are the components of the vector  $|\Psi'\rangle$  in our basis, we have from eqs. (A.12)–(A.15)

$$|\Psi'\rangle = A|\Psi\rangle = \sum_i \sum_j A_{ji} c_i |\chi_j\rangle = \sum_j d_j |\chi_j\rangle$$

and therefore

$$d_j = \sum_i A_{ji} c_i. \quad (\text{A.16})$$

This is a *matrix equation* which relates the components  $\{c_i\}$  of  $|\Psi\rangle$  and  $\{d_j\}$  of  $A|\Psi\rangle$  by means of the *matrix elements*  $A_{ji}$  of the linear operator  $A$ .

Given a linear, bounded, operator  $A$ , it is possible to define several new operators which are related to it. These are

i) The *adjoint* or *Hermitian conjugate* operator  $A^\dagger$  such that

$$(A^\dagger)_{ij} = A_{ji}^*. \quad (\text{A.17})$$

Hence, using eq. (A.14), we have

$$A_{ji} = \langle \chi_j | A | \chi_i \rangle = \langle \chi_i | A^\dagger | \chi_j \rangle^* = \langle A^\dagger \chi_j | \chi_i \rangle. \quad (\text{A.18})$$

We note that if  $|\Psi'\rangle = A|\Psi\rangle$ , then the conjugate bra of the vector  $|\Psi'\rangle$  is given by

$$\langle \Psi' | = \langle \Psi | A^\dagger. \quad (\text{A.19})$$

An operator  $A$  is called *Hermitian* if it is equal to its Hermitian conjugate. That is,

$$A = A^\dagger. \quad (\text{A.20})$$

The corresponding Hermitian matrix is therefore such that

$$A_{ij} = A_{ji}^*, \quad (\text{A.21})$$

or explicitly

$$\langle \chi_i | A | \chi_j \rangle = \langle \chi_j | A | \chi_i \rangle^*.$$

In particular, we note that for an Hermitian operator

$$\langle \chi_i | A | \chi_i \rangle = \langle \chi_i | A | \chi_i \rangle^* \quad (\text{A.22})$$

so that the quantity  $\langle \chi_i | A | \chi_i \rangle$  is real.

ii) The *transpose* of  $A$  is denoted by  $\tilde{A}$  and is defined by the relation

$$\tilde{A}_{ij} = A_{ji}. \quad (\text{A.23})$$

iii) The *inverse* operator  $A^{-1}$  of  $A$  is such that

$$A^{-1}A = AA^{-1} = I \quad (\text{A.24})$$

where  $I$  is the identity operator such that, for any vector  $|\Psi\rangle$  in the space, we have

$$I|\Psi\rangle = |\Psi\rangle. \quad (\text{A.25})$$

An Hermitian operator  $A$  is called a *projection operator* if

$$A^2 = A \cdot A = A. \quad (\text{A.26})$$

For example, let us consider a set of basis vectors  $\{\chi_i\}$  in a finite  $n$ -dimensional vector space. Then, using the unit operator  $I$ , we may write

$$I|\Psi\rangle = \sum_{i=1}^n |\chi_i\rangle\langle\chi_i|\Psi\rangle. \quad (\text{A.27})$$

Introducing the operators

$$A_i = |\chi_i\rangle\langle\chi_i| \quad (\text{A.28})$$

we see that

$$I = \sum_{i=1}^n A_i, \quad (\text{A.29})$$

and we verify that  $A_i^\dagger = A_i$ ,  $A_i^2 = A_i$  and  $A_i A_j = 0$  if  $i \neq j$ . Hence the operator  $A_i = |\chi_i\rangle\langle\chi_i|$  projects any vector into the one-dimensional subspace corresponding to the vector  $|\chi_i\rangle$ .

Finally, we define the *commutator* of two operators as

$$[A, B] = AB - BA \quad (\text{A.30})$$

while their *anticommutator* is given by

$$\{A, B\} = AB + BA. \quad (\text{A.31})$$

Two operators are said to *commute* when  $[A, B] = 0$ ; they *anticommute* if  $\{A, B\} = 0$ .

We now return to the principles of quantum mechanics. A fundamental postulate of quantum theory is that to every measurable property, i.e. to every *observable*  $\mathcal{A}$  (such as the position, momentum, energy, angular momentum, spin, etc.) of a system there corresponds an *Hermitian* operator. Let us call  $A$  the operator associated with the observable  $\mathcal{A}$ . We denote by  $\alpha_n$  the eigenvalues (or the elements of the *spectrum*) of this operator  $A$ , while  $|\Phi_n\rangle$  are the corresponding eigenvectors. Thus we write

$$A|\Phi_n\rangle = \alpha_n|\Phi_n\rangle. \quad (\text{A.32})$$

We observe that the eigenvalues  $\alpha_n$  of an Hermitian operator  $A$  are *real*. Indeed, we have from eq. (A.32)

$$\alpha_n = \frac{\langle\Phi_n|A|\Phi_n\rangle}{\langle\Phi_n|\Phi_n\rangle}. \quad (\text{A.33})$$



Moreover, the eigenvectors of  $A$  corresponding to *distinct* eigenvalues are orthogonal, since

$$(\alpha_n - \alpha_{n'})\langle \Phi_{n'} | \Phi_n \rangle = \langle \Phi_{n'} | A | \Phi_n \rangle - \langle A \Phi_{n'} | \Phi_n \rangle = 0 \quad (\text{A.34})$$

and therefore  $\langle \Phi_{n'} | \Phi_n \rangle = 0$  if  $\alpha_n \neq \alpha_{n'}$ . When all the eigenvalues are distinct they are said to be *non-degenerate*. On the contrary, they are *degenerate* when  $\alpha_n = \alpha_{n'}$  for  $n \neq n'$ . In that case the various eigenvectors  $\Phi_n^{(r)}$  which correspond to a given eigenvalue  $\alpha_n$  may be combined linearly so that they are orthogonal among themselves. Moreover, from eq. (A.34) we know that they are also orthogonal to the eigenvectors corresponding to other eigenvalues. We may thus choose all the eigenvectors  $|\Phi_n\rangle$  of the Hermitian operator  $A$  to be mutually orthogonal. We shall also normalize them in such a way that

$$\langle \Phi_{n'} | \Phi_n \rangle = \delta_{nn'} \quad \text{or} \quad \delta(n - n') \quad (\text{A.35})$$

and assume that they form a complete set. That is,

$$\sum_n |\Phi_n\rangle \langle \Phi_n| = 1 \quad (\text{A.36})$$

where the sum on  $n$  includes an integration over continuous variables, if necessary. We observe that in the orthonormal basis of its eigenvectors the operator  $A$  takes on the simple diagonal form

$$A = \sum_n |\Phi_n\rangle \alpha_n \langle \Phi_n| \quad (\text{A.37})$$

and we note that the operator

$$A_n = |\Phi_n\rangle \langle \Phi_n| \quad (\text{A.38})$$

is a projection operator onto the state  $\Phi_n$ . When there is no possible ambiguity it is convenient to use a simplified notation such that  $|\Phi_n\rangle \equiv |n\rangle$ ,  $\langle \Phi_n| \equiv \langle n|$ ,  $A_n = |n\rangle \langle n|$ , etc.

Functions of an observable  $F(\mathcal{A})$  lead to functions  $F(A)$  of an operator  $A$ . These may be defined with the help of the projection operators  $A_n$  as

$$F(A) = \sum_n F(\alpha_n) A_n = \sum_n |n\rangle F(\alpha_n) \langle n| \quad (\text{A.39})$$

provided that  $F(\alpha_n)$  exists for all eigenvalues  $\alpha_n$  of  $A$ .

Another basic postulate of quantum mechanics is that the only possible results of measurements performed on the system to determine the observable  $\mathcal{A}$  are the eigenvalues  $\alpha_n$  of the operator  $A$ . Furthermore, the probability that the system, described by the state vector  $|\Psi\rangle$ , gives the value  $\alpha_n$  for the observable  $\mathcal{A}$  is given by

$$P_n = |\langle \Phi_n | \Psi \rangle|^2 \quad (\text{A.40})$$

provided that the eigenvalue  $\alpha_n$  is *non-degenerate*. In other words, if we expand the state vector  $|\Psi\rangle$  in the basis  $\{\Phi_n\}$  as

$$|\Psi\rangle = \sum_n c_n |\Phi_n\rangle \quad (\text{A.41})$$

then the coefficients

$$c_n = \langle \Phi_n | \Psi \rangle \quad (\text{A.42})$$

are the *probability amplitudes* of finding the value  $\alpha_n$  for the observable  $\mathcal{A}$ . Immediately after a measurement which has given the value  $\alpha_n$  for the observable  $\mathcal{A}$ , we know that the state vector of the system is proportional to the eigenfunction  $|\Phi_n\rangle$  of  $A$ . Hence the measurement acts as a *filter*; it prepares the system in the state  $|\Phi_n\rangle$ .

If the eigenvalue  $\alpha_n$  is *degenerate*, the probability  $P_n$  of obtaining the value  $\alpha_n$  for the observable  $\mathcal{A}$  is now given by

$$P_n = \sum_r |\langle \Phi_n^{(r)} | \Psi \rangle|^2 \quad (\text{A.43})$$

where the sum runs over all values of the index  $r$  corresponding to the eigenvectors  $\Phi_n^{(r)}$  which belong to the degenerate eigenvalue  $\alpha_n$ . Before the measurement, the state vector may be written as

$$|\Psi\rangle = \sum_n \sum_r c_n^{(r)} |\Phi_n^{(r)}\rangle \quad (\text{A.44})$$

with

$$c_n^{(r)} = \langle \Phi_n^{(r)} | \Psi \rangle. \quad (\text{A.45})$$

After a measurement leading to the value  $\alpha_n$ , the system is described by the vector

$$|\Psi_n\rangle = \sum_r c_n^{(r)} |\Phi_n^{(r)}\rangle \quad (\text{A.46})$$

so that additional measurements must be carried out to ascertain the state of the system. It is another postulate of quantum mechanics that it is always possible to perform a set of simultaneous measurements which do not perturb each other and which specify uniquely the state of the system. Such measurements are said to form a *complete set of compatible measurements*. Two observables whose corresponding (Hermitian) operators commute can always be measured simultaneously (and vice-versa). A collection of commuting observables such that the simultaneous measurement of these observables specifies uniquely the state vector of the system is called a *complete set of (commuting) observables*. Hence a complete set of compatible measurements “prepares” the system (after the measurements) in a definite state [5]. Two observables described by non-commuting operators cannot be measured simultaneously (except for special states on which their commutator vanishes). For example, the position operator  $x$  and momentum operator  $p_x$ , which satisfy the commutation relation  $[x, p_x] = i\hbar$ , cannot be measured simultaneously. In fact, two canonically conjugate observables  $\mathcal{A}$  and  $\mathcal{B}$  whose corresponding operators  $A$  and  $B$  are such that

$$[A, B] = i\hbar \quad (\text{A.47})$$

satisfy the *Heisenberg uncertainty relation*

$$\Delta A \Delta B \geq \frac{1}{2}\hbar \quad (\text{A.48})$$

where

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2 \quad (\text{A.49})$$

is the mean square deviation about the expectation value of the observable for the system described by the state vector  $\Psi$ , namely

$$\langle A \rangle = \langle \Psi | A | \Psi \rangle. \quad (\text{A.50})$$

Similarly, we have

$$(\Delta B)^2 = \langle B^2 \rangle - \langle B \rangle^2. \quad (\text{A.51})$$

Particular cases of the relation (A.48) are the position-momentum uncertainty relation

$$\Delta x \Delta p_x \geq \frac{1}{2}\hbar \quad (\text{A.52})$$

and the time-energy uncertainty relation

$$\Delta t \Delta E \geq \frac{1}{2}\hbar. \quad (\text{A.53})$$

Let us now return to eq. (A.10). Having adopted a given *representation* (i.e. a complete orthonormal set of basis vectors  $\{\chi_i\}$ ), we have developed in it the state vector  $|\Psi\rangle$ . Likewise, the operator  $A$  is “represented” in this basis by its matrix elements (A.14). We may also develop the same vector  $|\Psi\rangle$  in the same space but in terms of another set of basis vectors  $\{\chi'_\lambda\}$  (i.e. in another representation) as

$$|\Psi\rangle = \sum_\lambda c'_\lambda |\chi'_\lambda\rangle. \quad (\text{A.54})$$

In particular, any “old” basis vector may be expressed in the “new” basis as

$$|\chi_i\rangle = \sum_\lambda U_{\lambda i} |\chi'_\lambda\rangle \quad (\text{A.55})$$

and therefore, since

$$|\Psi\rangle = \sum_i c_i |\chi_i\rangle = \sum_i \sum_\lambda c_i U_{\lambda i} |\chi'_\lambda\rangle = \sum_\lambda c'_\lambda |\chi'_\lambda\rangle \quad (\text{A.56})$$

we find that

$$c'_\lambda = \sum_i U_{\lambda i} c_i. \quad (\text{A.57})$$

Moreover, we note that because  $\langle \chi_j | \chi_i \rangle = \delta_{ij}$  and  $\langle \chi'_\mu | \chi'_\lambda \rangle = \delta_{\lambda\mu}$ , eq. (A.55) yields

$$UU^\dagger = U^\dagger U = I \quad (\text{A.58})$$

so that the operator  $U$  is *unitary*. Therefore the passage from one representation of quantum mechanics to another one is effected by a *unitary transformation*. Important representations of quantum mechanics are the *coordinate* or *position representation* (in which the coordinates of a particle are diagonal) and the *momentum representation* (in which the components of the momentum are diagonal).

Instead of changing the representation by means of a unitary transformation, we may also apply unitary transformations directly on the vectors and operators of Hilbert space. For example, let  $|\Psi\rangle$  and  $|\chi\rangle$  be two vectors such that

$$A|\Psi\rangle = |\chi\rangle. \quad (\text{A.59})$$

If we write

$$\begin{aligned} |\Psi'\rangle &= U|\Psi\rangle, \\ |\chi'\rangle &= U|\chi\rangle \end{aligned} \quad (\text{A.60})$$

and

$$A'|\Psi'\rangle = |\chi'\rangle$$

we find that  $A'U|\Psi\rangle = U|\chi\rangle = UA|\Psi\rangle$  and therefore

$$A = U^\dagger A' U; \quad A' = UAU^\dagger \quad (\text{A.61})$$

where we have used eq. (A.58). We note that such a unitary transformation leaves the system unchanged since

- i) The operator  $A'$  has the same eigenvalue spectrum as  $A$ ,
- ii) Operator equations remain unchanged,
- iii) The expectation values  $\langle\Psi|A|\Psi\rangle$  remain unchanged.

Of particular importance are the *infinitesimal unitary transformations*. Such transformations may be written in the form

$$U = I + i\varepsilon F \quad (\text{A.62})$$

where  $\varepsilon$  is a real, arbitrarily small parameter and the operator  $F$  must be *Hermitian*. Indeed, from eqs. (A.58) and (A.62) we deduce that to first order in  $\varepsilon$ ,

$$I = (I - i\varepsilon F^\dagger)(I + i\varepsilon F) \simeq I - i\varepsilon F^\dagger + i\varepsilon F \quad (\text{A.63})$$

so that  $\varepsilon(F - F^\dagger) = 0$  and

$$F = F^\dagger. \quad (\text{A.64})$$

We now consider the *time development of the system*. Let us imagine that the basis set which we have chosen in Hilbert space is fixed in time, so that the time evolution of the system is described by a time dependent state vector  $\Psi(t)$ . Such a description is said to be made in the *Schrödinger picture* [6]. It is then postulated that there exists an Hermitian operator  $H$ , called the Hamiltonian, which determines the time-development of the state vector  $\Psi$  according to the (time-dependent) *Schrödinger equation*

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H\Psi(t). \quad (\text{A.65})$$

We note that since eq. (A.65) is a first order differential equation in the time variable, the state vector  $\Psi(t)$  is determined for all values of  $t$  if it is given at one time  $t_0$ .

This ends our short survey of basic quantum mechanics. Detailed treatments of this subject may be found for example in the references [2, 7–9] listed at the end of this appendix.

## References and notes

- [1] A few useful references concerning vector spaces and Hilbert space are:  
 COURANT, R. and D. HILBERT (1953), *Methods of Mathematical Physics*, Vol. I (Interscience, New York) Chapters 1–3;  
 HALMOS, P. R. (1958), *Finite-Dimensional Vector Spaces* (second ed., Van Nostrand, Princeton);  
 HALMOS, P. R. (1951), *Introduction to Hilbert Space and the Theory of Spectral Multiplicity* (Chelsea, New York);  
 JACKSON, J. D. (1962), *Mathematics for Quantum Mechanics* (Benjamin, New York);  
 BYRON Jr., F. W. and R. W. FULLER (1969), *Mathematics of Classical and Quantum Physics*, Vol. I (Addison-Wesley, Reading, Mass.) Chapters 4, 5.
- [2] DIRAC, P. A. M. (1958), *The Principles of Quantum Mechanics* (fourth ed., Oxford University Press, New York).
- [3] We recall that in a finite  $n$ -dimensional vector space the scalar product of two vectors  $x$  and  $y$ , having respectively complex components  $(x_1, x_2, \dots, x_n)$  and  $(y_1, y_2, \dots, y_n)$ , is defined by

$$(x, y) \equiv \langle x | y \rangle = \sum_{i=1}^n x_i^* y_i$$

where the asterisk denotes complex conjugation. The natural extension of this definition to functions (i.e. members of infinite dimensional spaces) may be done as follows. Let us consider complex-valued functions  $f(x)$  of a real variable  $x$ , defined on a closed interval  $[a, b]$ . (The generalization to more variables is straightforward.) We shall assume that these functions are *square integrable*, i.e.  $\int_a^b |f(x)|^2 dx$  exists and is  $< \infty$ . Then the scalar product of two functions  $f_1$  and  $f_2$  is defined as

$$(f_1, f_2) \equiv \langle f_1 | f_2 \rangle \equiv \int_a^b f_1^*(x) f_2(x) dx.$$

- [4] WICK, G., A. WIGHTMAN and E. WIGNER (1952), *Phys. Rev.* **88**, 101.
- [5] In practice, it often happens that such “maximal” information about the system is not available. In this case the system is said to be in a mixed state; it cannot be described by a single state vector. Such systems are considered in Chapters 15 and 18.
- [6] Other “pictures” obtained by making unitary transformations on the state vector  $|\Psi\rangle$  are discussed in Chapter 13.
- [7] VON NEUMANN, J. (1955), *Mathematical Foundations of Quantum Mechanics* (Princeton University Press).
- [8] JAUCH, J. M. (1968), *Foundations of Quantum Mechanics* (Addison-Wesley, Reading, Mass.).
- [9] MESSIAH, A. (1968), *Quantum Mechanics* (Wiley, New York) Vol. I.

# Appendix B

## Legendre Polynomials, Associated Legendre Functions and Spherical Harmonics

### 1. Legendre polynomials

Let us consider the real variable  $x$  such that  $-1 \leq x \leq +1$ . We may also set  $x = \cos \theta$ , where  $\theta$  is a real number. The polynomials of degree  $l$  ( $l = 0, 1, 2, \dots$ )

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l \quad (\text{B.1})$$

are known as the *Legendre polynomials*. They satisfy the differential equation

$$\left[ (1 - x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx} + l(l + 1) \right] P_l(x) = 0. \quad (\text{B.2})$$

Furthermore,  $P_l(x)$  has the parity  $(-)^l$  and has  $l$  zeros in the interval  $(-1, +1)$ . A generating function for the Legendre polynomials is

$$\frac{1}{(1 - 2xt + t^2)^{1/2}} = \sum_{l=0}^{\infty} P_l(x) t^l, \quad |t| < 1. \quad (\text{B.3})$$

One also has the recurrence relations

$$(2l + 1)xP_l - (l + 1)P_{l+1} - lP_{l-1} = 0, \quad (\text{B.4a})$$

$$(x^2 - 1) \frac{dP_l}{dx} = l(xP_l - P_{l-1}) = \frac{l(l + 1)}{2l + 1} (P_{l+1} - P_{l-1}) \quad (\text{B.4b})$$

(also valid for  $l = 0$  if one defines  $P_{-1} = 0$ ). The orthogonality relations read

$$\int_{-1}^{+1} P_l(x) P_{l'}(x) dx = \frac{2}{2l + 1} \delta_{ll'}. \quad (\text{B.5})$$

One also has the closure relation

$$\frac{1}{2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) P_l(\cos \theta') = \delta(\cos \theta - \cos \theta'). \quad (\text{B.6})$$

Important particular values of the Legendre polynomials are

$$P_l(1) = 1, \quad P_l(-1) = (-1)^l. \quad (\text{B.7})$$

For the lowest values of  $l$  one has explicitly

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{1}{2}(3x^2 - 1) \\ P_3(x) &= \frac{1}{2}(5x^3 - 3x) \\ P_4(x) &= \frac{1}{8}(35x^4 - 30x^2 + 3). \end{aligned} \quad (\text{B.8})$$

## 2. Associated Legendre functions

These functions are defined by the relations

$$P_l^m(x) = (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_l(x), \quad m = 0, 1, 2, \dots, l, \quad (\text{B.9})$$

and we see that they are the product of the quantity  $(1 - x^2)^{m/2}$  and of a polynomial of degree  $(l - m)$  and parity  $(-1)^{l-m}$ , having  $(l - m)$  zeros in the interval  $(-1, +1)$ . The functions  $P_l^m$  satisfy the differential equation

$$\left[ (1 - x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx} + l(l+1) - \frac{m^2}{1 - x^2} \right] P_l^m(x) = 0 \quad (\text{B.10})$$

and they are given from a generating function as

$$(2m-1)!!(1-x^2)^{m/2} \frac{t^m}{(1-2xt+t^2)^{m+1/2}} = \sum_{l=m}^{\infty} P_l^m(x)t^l, \quad |t| < 1$$

with

$$(2m-1)!! = 1 \cdot 3 \cdot 5 \cdots (2m-1). \quad (\text{B.11})$$

In particular, one has

$$P_l^0(x) = P_l(x), \quad (\text{B.12})$$

$$P_l^l(x) = (2l-1)!!(1-x^2)^{l/2}. \quad (\text{B.13})$$

The functions  $P_l^m$  satisfy the recurrence relations

$$(2l+1)xP_l^m - (l-m+1)P_{l+1}^m - (l+m)P_{l-1}^m = 0, \quad (\text{B.14})$$

$$\begin{aligned} (x^2-1) \frac{dP_l^m}{dx} &= -(l+1)xP_l^m + (l-m+1)P_{l+1}^m \\ &= lxP_l^m - (l+m)P_{l-1}^m, \quad 0 \leq m \leq l-1, \end{aligned} \quad (\text{B.15})$$

$$P_l^{m+2} - 2(m+1)\frac{x}{(1-x^2)^{1/2}}P_l^{m+1} + (l-m)(l+m+1)P_l^m = 0, \quad 0 \leq m \leq l-2, \quad (\text{B.16})$$

$$P_{l-1}^m - P_{l+1}^m = -(2l+1)(1-x^2)^{1/2}P_l^{m-1}, \quad 0 \leq m \leq l-1 \quad (\text{B.17})$$

and the orthonormality relations

$$\int_{-1}^{+1} P_l^m(x) P_l^{m'}(x) dx = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'}. \quad (\text{B.18})$$

Important particular values are

$$P_l^m(1) = P_l^m(-1) = 0, \quad m \neq 0 \quad (\text{B.19})$$

[for  $m = 0$ , see eq. (B.7)]

$$P_l^m(0) = \begin{cases} (-)^s \frac{(2s+2m)!}{2^s s! (s+m)!}, & \text{if } l-m = 2s \\ 0, & \text{if } l-m = 2s+1. \end{cases} \quad (\text{B.20})$$

The first few associated Legendre functions are given explicitly by

$$\begin{aligned} P_1^1(x) &= (1-x^2)^{1/2}, \\ P_2^1(x) &= 3(1-x^2)^{1/2}x, \\ P_2^2(x) &= 3(1-x^2), \\ P_3^1(x) &= \frac{3}{2}(1-x^2)^{1/2}(5x^2-1), \\ P_3^2(x) &= 15x(1-x^2), \\ P_3^3(x) &= 15(1-x^2)^{3/2}. \end{aligned} \quad (\text{B.21})$$

### 3. Spherical harmonics

The spherical harmonics  $Y_{lm}(\theta, \phi)$  are eigenfunctions of the operators  $L^2$  and  $L_z$ . That is,

$$L^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}, \quad l = 0, 1, 2, \dots \quad (\text{B.22})$$

$$L_z Y_{lm} = m\hbar Y_{lm}, \quad m = -l, -l+1, \dots, l \quad (\text{B.23})$$

with

$$L_x = i\hbar \left( \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right), \quad (\text{B.24})$$

$$L_y = -i\hbar \left( \cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right), \quad (\text{B.25})$$

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \quad (\text{B.26})$$

and

$$L^2 = L_x^2 + L_y^2 + L_z^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]. \quad (\text{B.27})$$



One has [1]

$$Y_{lm}(\theta, \phi) = (-1)^m \left[ \frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\phi}, \quad m \geq 0 \quad (\text{B.28})$$

$$Y_{l,-m}(\theta, \phi) = (-1)^m Y_{lm}^*(\theta, \phi). \quad (\text{B.29})$$

The functions  $Y_{lm}$  have the parity  $(-)^l$ . Thus, in a reflection about the origin such that  $(\theta, \phi) \rightarrow (\pi - \theta, \phi + \pi)$ , one has

$$Y_{lm}(\pi - \theta, \phi + \pi) = (-)^l Y_{lm}(\theta, \phi). \quad (\text{B.30})$$

We also note that for  $m = 0$  and  $m = l$  the spherical harmonics are given respectively by the simple expressions

$$Y_{l,0}(\theta) = \left( \frac{2l+1}{4\pi} \right)^{1/2} P_l(\cos \theta) \quad (\text{B.31})$$

and

$$Y_{l,l}(\theta, \phi) = (-1)^l \left[ \frac{2l+1}{4\pi} \frac{(2l)!}{2^{2l}(l!)^2} \right]^{1/2} \sin^l \theta e^{il\phi}. \quad (\text{B.32})$$

The spherical harmonics satisfy the recurrence relations

$$\begin{aligned} L_{\pm} Y_{lm} &= \hbar[l(l+1) - m(m \pm 1)]^{1/2} Y_{l,m \pm 1}, \\ L_+ Y_{l,l} &= 0 \\ L_- Y_{l,-l} &= 0 \end{aligned} \quad (\text{B.33})$$

with

$$L_{\pm} = L_x \pm iL_y = \hbar e^{\pm i\phi} \left[ \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right]. \quad (\text{B.34})$$

The orthonormality relations are

$$\begin{aligned} \int Y_{l'm'}^*(\theta, \phi) Y_{lm}(\theta, \phi) d\Omega &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin \theta Y_{l'm'}^*(\theta, \phi) Y_{lm}(\theta, \phi) \\ &= \delta_{ll'} \delta_{mm'}, \quad (d\Omega = \sin \theta d\theta d\phi) \end{aligned} \quad (\text{B.35})$$

while the closure relation reads

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}^*(\theta, \phi) Y_{lm}(\theta', \phi') = \delta(\Omega - \Omega') \quad (\text{B.36})$$

with

$$\delta(\Omega - \Omega') = \frac{\delta(\theta - \theta') \delta(\phi - \phi')}{\sin \theta}. \quad (\text{B.37})$$

The first few spherical harmonics are given by

$$\begin{aligned} Y_{0,0} &= (4\pi)^{-1/2}, \\ Y_{1,0} &= \left( \frac{3}{4\pi} \right)^{1/2} \cos \theta, \\ Y_{1,1} &= -\left( \frac{3}{8\pi} \right)^{1/2} \sin \theta e^{i\phi}, \end{aligned}$$

$$\begin{aligned}
Y_{2,0} &= \left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1), \\
Y_{2,1} &= -\left(\frac{15}{8\pi}\right)^{1/2} \sin \theta \cos \theta e^{i\phi}, \\
Y_{2,2} &= \left(\frac{15}{32\pi}\right)^{1/2} \sin^2 \theta e^{2i\phi}, \\
Y_{3,0} &= \left(\frac{7}{16\pi}\right)^{1/2} (5 \cos^3 \theta - 3 \cos \theta), \\
Y_{3,1} &= -\left(\frac{21}{64\pi}\right)^{1/2} \sin \theta (5 \cos^2 \theta - 1) e^{i\phi}, \\
Y_{3,2} &= \left(\frac{105}{32\pi}\right)^{1/2} \sin^2 \theta \cos \theta e^{2i\phi}, \\
Y_{3,3} &= -\left(\frac{35}{64\pi}\right)^{1/2} \sin^3 \theta e^{3i\phi}.
\end{aligned} \tag{B.38}$$

#### 4. Some useful formulae

If  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are two vectors having polar angles  $(\theta_1, \phi_1)$  and  $(\theta_2, \phi_2)$ , and if we denote by  $\theta$  the angle between these two vectors, the “addition theorem” of spherical harmonics states that

$$P_l(\cos \theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y_{lm}^*(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2) \tag{B.39a}$$

or

$$P_l(\cos \theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y_{lm}^*(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \tag{B.39b}$$

where  $\hat{\mathbf{x}}$  denotes the polar angles of a vector  $\mathbf{x}$ .

Other useful relations are

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{(r_<)^l}{(r_>)^{l+1}} P_l(\cos \theta) \tag{B.40}$$

or

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} \frac{(r_<)^l}{(r_>)^{l+1}} Y_{lm}^*(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \tag{B.41}$$

where  $r_<$  is the smaller and  $r_>$  the larger of  $r_1$  and  $r_2$ . One also has

$$\frac{\exp\{ik|\mathbf{r}_1 - \mathbf{r}_2|\}}{|\mathbf{r}_1 - \mathbf{r}_2|} = ik \sum_{l=0}^{\infty} (2l+1) j_l(kr_<) h_l^{(1)}(kr_>) P_l(\cos \theta) \tag{B.42}$$

or

$$\frac{\exp\{ik|\mathbf{r}_1 - \mathbf{r}_2|\}}{|\mathbf{r}_1 - \mathbf{r}_2|} = 4\pi ik \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} j_l(kr_<) h_l^{(1)}(kr_>) Y_{lm}^*(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \quad (\text{B.43})$$

where  $j_l$  and  $h_l^{(1)}$  are respectively the spherical Bessel function and the spherical Hankel function of the first kind (see Appendix C).

The development in spherical harmonics of a plane wave  $\exp(i\mathbf{k} \cdot \mathbf{r})$  of wave vector  $\mathbf{k}$  is given by

$$\exp(i\mathbf{k} \cdot \mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}). \quad (\text{B.44})$$

Using the addition theorem (B.39), we may also write

$$\exp(i\mathbf{k} \cdot \mathbf{r}) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta) \quad (\text{B.45})$$

where  $\theta$  is the angle between the directions of the vectors  $\mathbf{k}$  and  $\mathbf{r}$ . In particular, if we choose the  $z$ -axis to coincide with the direction of  $\mathbf{k}$ , we have

$$\exp(i\mathbf{k} \cdot \mathbf{r}) \equiv e^{ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta). \quad (\text{B.46})$$

Finally, we quote the relation

$$\begin{aligned} & \int Y_{l_1, m_1}(\theta, \phi) Y_{l_2, m_2}(\theta, \phi) Y_{l_3, m_3}(\theta, \phi) d\Omega \\ &= \left[ \frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi} \right]^{1/2} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \end{aligned} \quad (\text{B.47})$$

where we have introduced the Wigner 3- $j$  symbols (see Appendix E). From eq. (B.47) one also finds that

$$\begin{aligned} Y_{l_1, m_1}(\theta, \phi) Y_{l_2, m_2}(\theta, \phi) &= \sum_{L=|l_1-l_2|}^{l_1+l_2} \sum_{M=-L}^L \left[ \frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)} \right]^{1/2} \\ &\times \langle l_1 l_2 00 | L0 \rangle \langle l_1 l_2 m_1 m_2 | LM \rangle Y_{L, M}(\theta, \phi) \end{aligned} \quad (\text{B.48})$$

where we have used vector addition coefficients (see Appendix E). This last equation may also be written in terms of Wigner 3- $j$  symbols as

$$\begin{aligned} Y_{l_1, m_1}(\theta, \phi) Y_{l_2, m_2}(\theta, \phi) &= \sum_{L=|l_1-l_2|}^{l_1+l_2} \sum_{M=-L}^{+L} (-1)^M \\ &\times \left[ \frac{(2l_1+1)(2l_2+1)(2L+1)}{4\pi} \right]^{1/2} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} Y_{L, -M}(\theta, \phi). \end{aligned} \quad (\text{B.49})$$

Additional useful formulae involving the Legendre polynomials, associated Legendre functions and spherical harmonics may be found in the references [2–5]. We have followed here the conventions used in ref. [5].

## References and notes

- [1] The equations (B.22)–(B.23) and (B.35) determine the functions  $Y_{lm}(\theta, \phi)$  up to a phase. The choice of phase made in writing down the relations (B.28)–(B.29) ensures that
  - i) The functions  $Y_{lm}$  obtained in this way verify the recurrence relations (B.33)
  - ii)  $Y_{l,0}(0, 0)$  is real and positive.
 Since different authors choose different phase factor conventions for the spherical harmonics, one should be careful to check this point in dealing with the functions  $Y_{lm}$  used in the physics literature.
- [2] ABRAMOWITZ, M. and I. A. STEGUN (1965), *Handbook of Mathematical Functions* (Dover Publ., New York) Chapter 8.
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- [5] EDMONDS, A. R. (1957), *Angular Momentum in Quantum Mechanics* (Princeton University Press) Chapter 2.

# Appendix C

## Spherical Bessel Functions

Let us consider the differential equation (4.20), namely

$$\left[ \frac{d^2}{dz^2} + \frac{2}{z} \frac{d}{dz} + \left( 1 - \frac{l(l+1)}{z^2} \right) \right] f_l = 0 \quad (\text{C.1})$$

with  $l = 0, 1, 2, \dots$ . Particular solutions of this equation are:

i) The (genuine) *spherical Bessel functions* (or spherical Bessel functions of the first kind)

$$j_l(z) = \left( \frac{\pi}{2z} \right)^{1/2} J_{l+1/2}(z) \quad (\text{C.2})$$

where  $J_\nu(z)$  is an ordinary Bessel function of order  $\nu$ . The functions  $j_l(z)$  are *regular* at the origin [see eq. (C.11a)].

ii) *The spherical Neumann functions*

$$n_l(z) = (-1)^{l+1} \left( \frac{\pi}{2z} \right)^{1/2} J_{-l-1/2}(z) \quad (\text{C.3})$$

which are *irregular* solutions of eq. (C.1)

iii) The *spherical Hankel functions* of the first and second kind

$$h_l^{(1)}(z) = j_l(z) + in_l(z) \quad (\text{C.4})$$

and

$$h_l^{(2)}(z) = j_l(z) - in_l(z) \quad (\text{C.5})$$

which are *irregular* solutions of eq. (C.1). Thus

$$j_l(z) = \frac{1}{2} [h_l^{(1)}(z) + h_l^{(2)}(z)] \quad (\text{C.6})$$

and

$$n_l(z) = \frac{1}{2l} [h_l^{(1)}(z) - h_l^{(2)}(z)]. \quad (\text{C.7})$$

The pairs  $\{j_l(z), n_l(z)\}$  and  $\{h_l^{(1)}(z), h_l^{(2)}(z)\}$  are linearly independent solutions of eq. (C.1) for every  $l$ .

The first three functions  $j_l$  and  $n_l$  are given explicitly by

$$\begin{aligned} j_0(z) &= \frac{\sin z}{z}, \\ j_1(z) &= \frac{\sin z}{z^2} - \frac{\cos z}{z}, \\ j_2(z) &= \left(\frac{3}{z^3} - \frac{1}{z}\right) \sin z - \frac{3}{z^2} \cos z \end{aligned} \quad (\text{C.8})$$

and

$$\begin{aligned} n_0(z) &= -\frac{\cos z}{z}, \\ n_1(z) &= -\frac{\cos z}{z^2} - \frac{\sin z}{z}, \\ n_2(z) &= -\left(\frac{3}{z^3} - \frac{1}{z}\right) \cos z - \frac{3}{z^2} \sin z. \end{aligned} \quad (\text{C.9})$$

The functions  $j_0(x)$ ,  $j_1(x)$ ,  $j_2(x)$  and  $n_0(x)$ ,  $n_1(x)$ ,  $n_2(x)$ , where  $x$  is real, are plotted in Figs. C.1 and C.2.

The functions  $j_l(z)$  and  $n_l(z)$  may be represented by the ascending series [1-3]

$$j_l(z) = \frac{z^l}{(2l+1)!!} \left[ 1 - \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{(\frac{1}{2}z^2)^2}{2!(2l+3)(2l+5)} - \cdots \right] \quad (\text{C.10a})$$

$$n_l(z) = -\frac{(2l-1)!!}{z^{l+1}} \left[ 1 - \frac{\frac{1}{2}z^2}{1!(1-2l)} + \frac{(\frac{1}{2}z^2)^2}{2!(1-2l)(3-2l)} - \cdots \right] \quad (\text{C.10b})$$

where

$$(2l+1)!! = 1 \cdot 3 \cdot 5 \cdots (2l+1).$$

We see from eqs. (C.10) that for  $z \rightarrow 0$  one has

$$z^{-l} j_l(z) \xrightarrow{z \rightarrow 0} \frac{1}{(2l+1)!!}; \quad j_l(z) \underset{z \rightarrow 0}{\sim} \frac{z^l}{(2l+1)!!}, \quad (\text{C.11a})$$

$$z^{l+1} n_l(z) \xrightarrow{z \rightarrow 0} -(2l-1)!!; \quad n_l(z) \underset{z \rightarrow 0}{\sim} -\frac{(2l-1)!!}{z^{l+1}}. \quad (\text{C.11b})$$

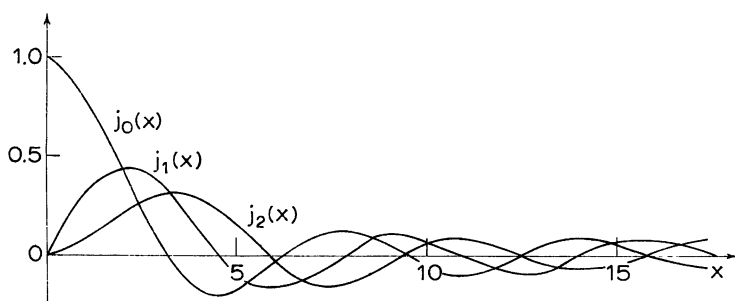


Fig. C.1. The first three spherical Bessel functions.

For real  $x$  somewhat larger than  $l(l+1)$  one may use the asymptotic formulae

$$j_l(x) \rightarrow \frac{1}{x} \sin(x - \tfrac{1}{2}l\pi), \quad (\text{C.12a})$$

$$n_l(x) \rightarrow -\frac{1}{x} \cos(x - \tfrac{1}{2}l\pi), \quad (\text{C.12b})$$

$$h_l^{(1)}(x) \rightarrow -i \frac{\exp\{i(x - \tfrac{1}{2}l\pi)\}}{x}, \quad (\text{C.12c})$$

$$h_l^{(2)}(x) \rightarrow i \frac{\exp\{-i(x - \tfrac{1}{2}l\pi)\}}{x}. \quad (\text{C.12d})$$

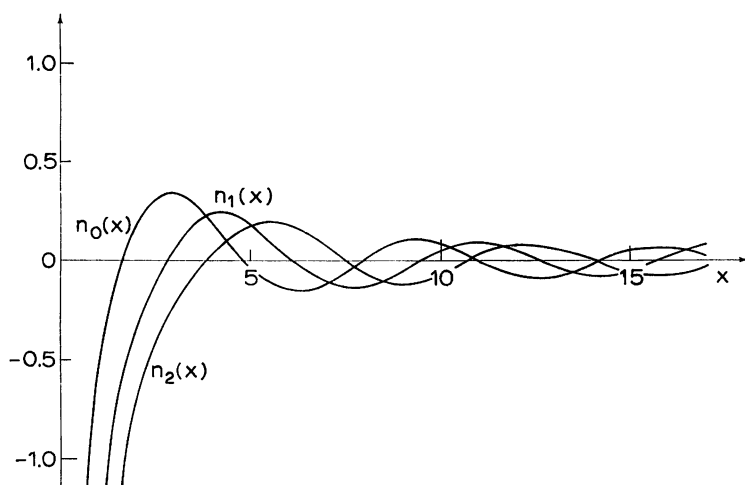


Fig. C.2. The first three spherical Neumann functions.

Some important properties of the spherical Bessel functions  $f_l$  [with  $f_l : j_l, n_l, h_l^{(1)}, h_l^{(2)}$ ] are the recurrence relations (we assume that  $l > 0$ )

$$f_{l-1}(z) + f_{l+1}(z) = \frac{2l+1}{z} f_l(z), \quad (\text{C.13a})$$

$$\frac{d}{dz} f_l(z) = \frac{1}{2l+1} [l f_{l-1}(z) - (l+1) f_{l+1}(z)] \quad (\text{C.13b})$$

$$f_{l-1}(z) = \frac{l+1}{z} f_l(z) + \frac{d}{dz} f_l(z) \quad (\text{C.13c})$$

$$f_{l+1}(z) = \frac{l}{z} f_l(z) - \frac{d}{dz} f_l(z). \quad (\text{C.13d})$$

One also has the differentiation formulae

$$\frac{d}{dz} [z^{l+1} f_l(z)] = z^{l+1} f_{l-1}(z), \quad (\text{C.14a})$$

$$\frac{d}{dz} [z^{-l} f_l(z)] = -z^{-l} f_{l+1}(z) \quad (\text{C.14b})$$

and the analytic continuations (with  $l, m = 0, 1, 2, \dots$ )

$$j_l(z e^{m\pi i}) = e^{ml\pi i} j_l(z), \quad (\text{C.15a})$$

$$n_l(z e^{m\pi i}) = (-1)^m e^{ml\pi i} n_l(z), \quad (\text{C.15b})$$

$$h_l^{(1)}(z e^{(2m+1)\pi i}) = (-1)^l h_l^{(2)}(z), \quad (\text{C.15c})$$

$$h_l^{(2)}(z e^{(2m+1)\pi i}) = (-1)^l h_l^{(1)}(z), \quad (\text{C.15d})$$

$$h_l^{(k)}(z e^{2m\pi i}) = h_l^{(k)}(z), \quad k = 1, 2. \quad (\text{C.15e})$$

In particular, we see that

$$j_l(-z) = (-1)^l j_l(z), \quad (\text{C.16a})$$

$$n_l(-z) = (-1)^{l+1} n_l(z), \quad (\text{C.16b})$$

$$h_l^{(1)}(-z) = (-1)^l h_l^{(2)}(z), \quad (\text{C.16c})$$

$$h_l^{(2)}(-z) = (-1)^l h_l^{(1)}(z). \quad (\text{C.16d})$$

Additional useful properties of the functions  $j_l$  and  $n_l$  are

$$j_l(z) n_{l-1}(z) - j_{l-1}(z) n_l(z) = z^{-2}, \quad l > 0 \quad (\text{C.17a})$$

$$j_l(z) \frac{d}{dz} n_l(z) - n_l(z) \frac{d}{dz} j_l(z) = z^{-2} \quad (\text{C.17b})$$

$$\int j_0^2(x) x^2 dx = \frac{1}{2} x^3 [j_0^2(x) + n_0(x) j_1(x)] \quad (\text{C.17c})$$

$$\int n_0^2(x) x^2 dx = \frac{1}{2} x^3 [n_0^2(x) - j_0(x) n_1(x)] \quad (\text{C.17d})$$

$$\int j_1(x) dx = -j_0(x) \quad (\text{C.17e})$$

$$\int j_0(x) x^2 dx = x^2 j_1(x) \quad (\text{C.17f})$$

$$\int j_l^2(x) x^2 dx = \frac{1}{2} x^3 [j_l^2(x) - j_{l-1}(x) j_{l+1}(x)], \quad l > 0. \quad (\text{C.17g})$$



The last three formulae are equally valid with the  $j$ 's replaced by the corresponding  $n$ 's.

Let us also quote a few definite integrals [4] involving the functions  $j_l$  and which are often used in scattering theory calculations, namely

$$\int_0^\infty e^{-ax} j_l(bx) x^{\mu-1} dx = \frac{\sqrt{\pi} b^l \Gamma(\mu + l)}{2^{l+1} a^{\mu+l} \Gamma(l + \frac{3}{2})} \\ \times {}_2F_1\left(\frac{\mu + l}{2}, \frac{\mu + l + 1}{2}; l + \frac{3}{2}; -\frac{b^2}{a^2}\right) \\ (\operatorname{Re}(a + ib) > 0, \operatorname{Re}(a - ib) > 0, \operatorname{Re}(\mu + l) > 0), \quad (\text{C.18a})$$

$$\int_0^\infty e^{-ax} j_l(bx) x^{l+1} dx = \frac{(2b)^l \Gamma(l + 1)}{(a^2 + b^2)^{l+1}} \quad (\operatorname{Re} a > |\operatorname{Im} b|), \quad (\text{C.18b})$$

$$\int_0^\infty e^{-ax} j_l(bx) x^{l+2} dx = \frac{2a (2b)^l \Gamma(l + 2)}{(a^2 + b^2)^{l+2}} \quad (\operatorname{Re} a > |\operatorname{Im} b|). \quad (\text{C.18c})$$

Similar integrals involving higher powers of  $x$  may be obtained by differentiating with respect to the quantity  $a$ .

Finally, we note that

$$\int_0^\infty j_l(kr) j_l(k'r) r^2 dr = \frac{\pi}{2k^2} \delta(k - k'). \quad (\text{C.19})$$

## References

- [1] WHITTAKER, E. T. and G. N. WATSON (1952), *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England).
- [2] WATSON, G. N. (1945), *Treatise on the Theory of Bessel functions* (2nd ed., MacMillan, New York).
- [3] ABRAMOWITZ, M. and I. A. STEGUN (1965), *Handbook of Mathematical Functions* (Dover Publ., New York) Chapter 10.
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# Appendix D

## Dalitz Integrals

Let us consider Dalitz integrals [1] of the type

$$I_{m,n}(\alpha, \beta; \mathbf{k}_i, \mathbf{k}_f; k) = \int d\mathbf{k} \frac{1}{\kappa^2 - k^2 - i\varepsilon} \frac{1}{(\alpha^2 + |\mathbf{k} - \mathbf{k}_i|^2)^m (\beta^2 + |\mathbf{k} - \mathbf{k}_f|^2)^n} \quad (m, n = 1, 2, \dots). \quad (D.1)$$

We first set

$$\begin{aligned} a &= \alpha^2 + |\mathbf{k} - \mathbf{k}_i|^2 \\ b &= \beta^2 + |\mathbf{k} - \mathbf{k}_f|^2, \end{aligned} \quad (D.2)$$

and use the Feynman integral representations [2]

$$\begin{aligned} \frac{1}{ab} &= \int_0^1 \frac{dt}{[at + b(1-t)]^2} \\ \frac{1}{a^2b} &= 2 \int_0^1 \frac{t}{[at + b(1-t)]^3} dt \\ &\vdots \\ \frac{1}{a^m b^n} &= \frac{(m+n-1)!}{(m-1)!(n-1)!} \int_0^1 \frac{t^{m-1}(1-t)^{n-1}}{[at + b(1-t)]^{m+n}} dt \end{aligned} \quad (D.3)$$

to write

$$\begin{aligned} I_{m,n}(\alpha, \beta; \mathbf{k}_i, \mathbf{k}_f; k) &= \frac{(m+n-1)!}{(m-1)!(n-1)!} \int_0^1 dt t^{m-1}(1-t)^{n-1} \\ &\quad \times \int d\mathbf{k} \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\Gamma^2 + |\mathbf{k} - \mathbf{\Lambda}|^2)^{m+n}} \end{aligned} \quad (D.4)$$

where we have set

$$\Gamma^2 = \alpha^2 t + \beta^2(1-t) + t(1-t)|\mathbf{k}_i - \mathbf{k}_f|^2 \quad (D.5)$$

and

$$\Lambda = tk_i + (1 - t)k_f. \quad (\text{D.6})$$

Apart from a one-dimensional integral on the  $t$  variable, the calculation of  $I_{m,n}(\alpha, \beta; k_i, k_f; k)$  therefore reduces to the evaluation of integrals of the type

$$L_S(k, \Gamma, \Lambda) = \int d\kappa \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\Gamma^2 + |\kappa - \Lambda|^2)^S}.$$

Let us start from the simple case  $S = 1$  for which

$$L_1(k, \Gamma, \Lambda) = \int d\kappa \frac{1}{(\kappa^2 - k^2 - i\varepsilon)(\Gamma^2 + |\kappa - \Lambda|^2)}. \quad (\text{D.7})$$

We take  $\Lambda$  as the  $z$ -axis of spherical coordinates  $(\kappa, \theta_\kappa, \varphi_\kappa)$  in  $\kappa$  space. Performing the integration over the azimuthal angle  $\varphi_\kappa$ , we find that

$$L_1 = 2\pi \int_0^\pi \sin \theta_\kappa d\theta_\kappa \times \int_0^\infty \frac{\kappa^2}{(\kappa^2 - k^2 - i\varepsilon)(\Gamma^2 + \kappa^2 + \Lambda^2 - 2\kappa\Lambda \cos \theta_\kappa)} d\kappa. \quad (\text{D.8})$$

Changing the variables of integration in eq. (D.8) to  $\theta'_\kappa = \pi - \theta_\kappa$  and  $\kappa' = -\kappa$ , we can also write

$$L_1 = 2\pi \int_0^\pi \sin \theta'_\kappa d\theta'_\kappa \times \int_{-\infty}^0 \frac{\kappa'^2}{(\kappa'^2 - k^2 - i\varepsilon)(\Gamma^2 + \kappa'^2 + \Lambda^2 - 2\kappa'\Lambda \cos \theta'_\kappa)} d\kappa'. \quad (\text{D.9})$$

Therefore, from eqs. (D.8) and (D.9), we deduce that

$$L_1 = \pi \int_0^\pi \sin \theta_\kappa d\theta_\kappa \times \int_{-\infty}^{+\infty} \frac{\kappa^2}{(\kappa^2 - k^2 - i\varepsilon)(\Gamma^2 + \kappa^2 + \Lambda^2 - 2\kappa\Lambda \cos \theta_\kappa)} d\kappa. \quad (\text{D.10})$$

Let us perform the integral on the variable  $\kappa$  by closing the contour with a semi-circle of infinite radius in the upper-half complex  $\kappa$  plane. The poles of the denominator in this upper-half plane occur at

$$\kappa_1 = k + i\varepsilon \quad \text{and} \quad \kappa_2 = \Lambda \cos \theta_\kappa + i\sqrt{\Gamma^2 + \Lambda^2 \sin^2 \theta_\kappa}. \quad (\text{D.11})$$

Hence, using the residue theorem, we find that

$$L_1 = \pi^2 i k \int_{-1}^{+1} \frac{d\omega}{\Gamma^2 + k^2 + \Lambda^2 - 2k\Lambda\omega} + \frac{\pi^2 i}{\Lambda} \int_{i\Gamma-\Lambda}^{i\Gamma+\Lambda} \frac{\kappa_2}{\kappa_2^2 - k^2 - i\varepsilon} d\kappa_2 \quad (\text{D.12})$$

where we have set  $\omega = \cos \theta_*$  in the first integral. Therefore,

$$L_1(k, \Gamma, \Lambda) = \frac{\pi^2 i}{\Lambda} \log \left( \frac{k + \Lambda + i\Gamma}{k - \Lambda + i\Gamma} \right). \quad (\text{D.13})$$

By successive differentiations with respect to  $\Gamma$ , we see that

$$\begin{aligned} L_2(k, \Gamma, \Lambda) &= - \frac{\pi^2}{\Gamma(k^2 - \Gamma^2 - \Lambda^2 + 2ik\Gamma)} \\ &\vdots \\ L_S(k, \Gamma, \Lambda) &= - \frac{1}{2(S-1)\Gamma} \frac{\partial L_{S-1}}{\partial \Gamma}. \end{aligned} \quad (\text{D.14})$$

With the quantities  $L_S$  obtained in this way, we may now return to eq. (D.4) which reads

$$I_{m,n}(\alpha, \beta; k_i, k_f; k) = \frac{(m+n-1)!}{(m-1)!(n-1)!} \int_0^1 t^{m-1} (1-t)^{n-1} L_{m+n}(k, \Gamma, \Lambda) dt \quad (\text{D.15})$$

where the objects  $\Gamma$  and  $\Lambda$  depend on  $t$  via the relations (D.5) and (D.6), respectively.

In certain cases simple closed form expressions may be obtained for the integration on the variable  $t$ . For example, if we consider the expression (8.95) which gives the quantity  $\tilde{f}_{B2}$  for a simple Yukawa potential of the form (8.81), we see that

$$\tilde{f}_{B2} = (2\pi^2)^{-1} U_0^2 I_{1,1}(\alpha, \alpha; k_i, k_f; k) \quad (\text{D.16})$$

or

$$\tilde{f}_{B2} = (2\pi^2)^{-1} U_0^2 \int_0^1 dt \int d\mathbf{k} \frac{1}{\kappa^2 - k^2 - i\epsilon} \frac{1}{[\Gamma^2 + |\mathbf{k} - \Lambda|^2]^2}. \quad (\text{D.17})$$

Since  $|k_i| = |k_f| = k$  and  $\alpha = \beta$  in this case, we have

$$\Gamma^2 + \Lambda^2 = k^2 + \alpha^2 \quad (\text{D.18})$$

so that, using the first of eqs. (D.14), we have

$$\tilde{f}_{B2} = -\frac{1}{2} U_0^2 \int_0^1 \frac{dt}{\Gamma(-\alpha^2 + 2ik\Gamma)}. \quad (\text{D.19})$$

Because  $\Gamma^2$  is a simple algebraic function of  $t$ , the integral (D.19) can be done in closed form to yield

$$\begin{aligned} \tilde{f}_{B2}(k, \theta) &= \frac{U_0^2}{2k \sin \frac{1}{2}\theta [\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2}} \\ &\times \left\{ \tan^{-1} \frac{\alpha k \sin \frac{1}{2}\theta}{[\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2}} \right. \\ &\left. + \frac{1}{2} i \log \left[ \frac{[\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2} + 2k^2 \sin \frac{1}{2}\theta}{[\alpha^4 + 4k^2(\alpha^2 + k^2 \sin^2 \frac{1}{2}\theta)]^{1/2} - 2k^2 \sin \frac{1}{2}\theta} \right] \right\} \quad (\text{D.20}) \end{aligned}$$

where  $\theta$  is the angle between the vectors  $k_i$  and  $k_f$ . This is precisely the result quoted in eq. (8.98).

## *References*

- [1] DALITZ, R. H. (1951), Proc. Roy. Soc. **A206**, 509; see also  
MORSE, P. M. and H. FESHBACH (1953), *Methods of Theoretical Physics* (McGraw-Hill, New York) Chapter 9.
- [2] FEYNMAN, R. P. (1949), Phys. Rev. **76**, 769, Appendix.

# Appendix E

## Vector Addition Coefficients and 3-j

### Symbols

Let us consider two quantum systems having angular momenta  $\mathbf{J}_1$  and  $\mathbf{J}_2$ , respectively. We denote by  $|j_1, m_1\rangle$  the eigenvectors of the system 1 common to the operators  $\mathbf{J}_1^2$  and  $J_{1,z}$  (the z-component of  $\mathbf{J}_1$ ). Thus

$$\begin{aligned} \mathbf{J}_1^2 |j_1, m_1\rangle &= j_1(j_1 + 1)\hbar^2 |j_1, m_1\rangle, \\ J_{1,z} |j_1, m_1\rangle &= m_1\hbar |j_1, m_1\rangle \end{aligned} \quad (\text{E.1})$$

where

$$m_1 = -j_1, -j_1 + 1, \dots, j_1.$$

Similarly, we have

$$\begin{aligned} \mathbf{J}_2^2 |j_2, m_2\rangle &= j_2(j_2 + 1)\hbar^2 |j_2, m_2\rangle, \\ J_{2,z} |j_2, m_2\rangle &= m_2\hbar |j_2, m_2\rangle \end{aligned} \quad (\text{E.2})$$

with

$$m_2 = -j_2, -j_2 + 1, \dots, j_2.$$

Simultaneous eigenvectors of the operators  $\mathbf{J}_1^2, J_{1,z}, \mathbf{J}_2^2$  and  $J_{2,z}$  are then given by the tensor product

$$|j_1 m_1 j_2 m_2\rangle = |j_1, m_1\rangle |j_2, m_2\rangle. \quad (\text{E.3})$$

We now consider the total angular momentum

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \quad (\text{E.4})$$

with components  $J_x, J_y, J_z$ . Since the operators  $\mathbf{J}_1^2$  and  $\mathbf{J}_2^2$  commute with  $\mathbf{J}$ , the eigenvectors of  $\mathbf{J}^2$  and  $J_z$  may be found among those of  $\mathbf{J}_1^2$  and  $\mathbf{J}_2^2$ . They will therefore be denoted as  $|j_1 j_2 jm\rangle$ , and one has [1, 2]

$$\begin{aligned} \mathbf{J}^2 |j_1 j_2 jm\rangle &= j(j + 1)\hbar^2 |j_1 j_2 jm\rangle \\ \text{and} \quad J_z |j_1 j_2 jm\rangle &= m\hbar |j_1 j_2 jm\rangle \end{aligned} \quad (\text{E.5})$$

with

$$j = |j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2 \quad (\text{E.6})$$

and

$$m = -j, -j + 1, \dots, +j.$$

The  $(2j_1 + 1)(2j_2 + 1)$  eigenvectors  $|j_1 j_2 jm\rangle$  common to the operators  $J_1^2, J_2^2, J^2, J_z$  are related to the  $(2j_1 + 1)(2j_2 + 1)$  eigenvectors  $|j_1 m_1 j_2 m_2\rangle$  common to the operators  $J_1^2, J_{1z}, J_2^2, J_{2z}$  by the unitary transformation

$$|j_1 j_2 jm\rangle = \sum_{m_1, m_2} \langle j_1 j_2 m_1 m_2 | jm \rangle |j_1 m_1 j_2 m_2\rangle. \quad (\text{E.7})$$

The coefficients  $\langle j_1 j_2 m_1 m_2 | jm \rangle$  of this transformation are called *vector addition coefficients*, *Wigner coefficients* [3] or *Clebsch–Gordan coefficients*. To define these coefficients unambiguously, the relative phases of the eigenvectors  $|j_1 m_1 j_2 m_2\rangle$  and  $|j_1 j_2 jm\rangle$  must be specified. The most frequently used convention is that of Condon and Shortley [4], namely

i) If  $J_{\pm} = J_x \pm iJ_y$ , then

$$J_{\pm} |j_1 j_2 jm\rangle = \hbar[j(j+1) - m(m \pm 1)]^{1/2} |j_1 j_2 jm \pm 1\rangle \quad (\text{E.8})$$

with similar relationships for  $|j_1, m_1\rangle$  and  $|j_2, m_2\rangle$ .

ii)  $\langle j_1 j_2 j_1(j_1 - j) | j j \rangle$  is real and positive. (E.9)

We note that the vector addition coefficients vanish unless  $|j_1 - j_2| \leq j \leq j_1 + j_2$  and  $m = m_1 + m_2$ . Moreover, with the phase conventions adopted above, the vector addition coefficients are *real*. Some important properties of these coefficients are

1) *Orthogonality relations*

$$\sum_{m_1, m_2} \langle j_1 j_2 m_1 m_2 | jm \rangle \langle j_1 j_2 m_1 m_2 | j' m' \rangle = \delta_{jj'} \delta_{mm'} \quad (\text{E.10})$$

$$\sum_{j, m} \langle j_1 j_2 m_1 m_2 | jm \rangle \langle j_1 j_2 m'_1 m'_2 | jm \rangle = \delta_{m_1 m'_1} \delta_{m_2 m'_2}. \quad (\text{E.11})$$

2) *Symmetry properties*

$$\langle j_1 j_2 m_1 m_2 | jm \rangle = (-)^{j_1 + j_2 - j} \langle j_2 j_1 m_2 m_1 | jm \rangle \quad (\text{E.12})$$

$$= (-)^{j_1 + j_2 - j} \langle j_1 j_2 - m_1 - m_2 | j - m \rangle \quad (\text{E.13})$$

$$= \langle j_2 j_1 - m_2 - m_1 | j - m \rangle \quad (\text{E.14})$$

$$= (-)^{j_1 - m_1} \left( \frac{2j + 1}{2j_2 + 1} \right)^{1/2} \langle j_1 j_1 m_1 - m | j_2 - m_2 \rangle \quad (\text{E.15})$$

$$= (-)^{j_2 + m_2} \left( \frac{2j + 1}{2j_1 + 1} \right)^{1/2} \langle j j_2 - m m_2 | j_1 - m_1 \rangle. \quad (\text{E.16})$$

The symmetry properties can be expressed in a particularly simple way by using the *Wigner 3-j symbols* defined by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-)^{j_1 - j_2 - m_3} (2j_3 + 1)^{-1/2} \langle j_1 j_2 m_1 m_2 | j_3 - m_3 \rangle. \quad (\text{E.17})$$

Indeed, the 3- $j$  symbol is invariant for an even number of permutations of the columns; it is multiplied by  $(-)^{j_1+j_2+j_3}$  for an odd number of permutations or when one changes the sign of the three numbers  $m_1, m_2, m_3$ . Thus

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix} \\ &= (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} \end{aligned} \quad (\text{E.18})$$

and

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (\text{E.19})$$

The orthogonality relations for the 3- $j$  symbols read [5]

$$\sum_{m_1, m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j'_3 \\ m_1 & m_2 & m'_3 \end{pmatrix} = \varepsilon(j_1 j_2 j_3) (2j_3 + 1)^{-1} \delta_{j_3 j'_3} \delta_{m_3 m'_3}, \quad (\text{E.20})$$

$$\sum_{j_3, m_3} (2j_3 + 1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m_3 \end{pmatrix} = \varepsilon(j_1 j_2 j_3) \delta_{m_1 m'_1} \delta_{m_2 m'_2}, \quad (\text{E.21})$$

$$\sum_{m_1, m_2, m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \varepsilon(j_1 j_2 j_3) \quad (\text{E.22})$$

where

$$\varepsilon(j_1 j_2 j_3) = \begin{cases} 1, & \text{if } |j_1 - j_2| \leq j_3 \leq j_1 + j_2 \\ 0, & \text{otherwise.} \end{cases}$$

Details concerning the explicit computation of the vector addition coefficients and the 3- $j$  symbols, together with recursion relations and tables, are given for example in Ref. [6].

## References

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- [2] MESSIAH, A. (1968), *Quantum Mechanics* (Wiley, New York) Vol. II, Chapter 13 and Appendix C.
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- [5] See for example de SHALIT, A. and I. TALMI (1963), *Nuclear Shell Theory* (Academic Press, New York and London).
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# Appendix F

## The Wigner Simplified Rotation Matrices

The Wigner simplified rotation matrices  $d_{M'M}^J(\beta)$  are given by [1]

$$d_{M'M}^J(\beta) = [(J+M)!(J-M)!(J+M')!(J-M')!]^{1/2} \times \sum_{\kappa} \frac{(-)^{\kappa}}{(J-M'-\kappa)!(J+M-\kappa)!(\kappa+M'-M)! \kappa!} \times (\cos \frac{1}{2}\beta)^{2J+M-M'-2\kappa} (-\sin \frac{1}{2}\beta)^{M'-M+2\kappa} \quad (\text{F.1})$$

where the sum runs over values of the integer  $\kappa$  such that the arguments in the factorials are non-negative. Eq. (F.1) may also be written as [2]

$$d_{M'M}^J(\beta) = \left\{ \frac{(J+M)!(J-M)!}{(J+M')!(J-M')!} \right\}^{1/2} (\cos \frac{1}{2}\beta)^{M+M'} (\sin \frac{1}{2}\beta)^{M-M'} \times P_{J-M}^{(M-M', M+M')}(\cos \beta). \quad (\text{F.2})$$

Here  $P_n^{(\alpha, \gamma)}$  are Jacobi polynomials [3] which are particular cases of the hypergeometric function. That is,

$$P_n^{(\alpha, \gamma)}(x) = \binom{n+\alpha}{n} {}_2F_1(-n, n+\alpha+\gamma+1; \alpha+1; \frac{1}{2}-\frac{1}{2}x) \quad (\text{F.3})$$

where

$$\binom{n+\alpha}{n} = \frac{(n+\alpha)(n+\alpha-1)\cdots(\alpha+1)}{1\cdot 2\cdots n} \quad (\text{F.4})$$

and

$${}_2F_1(a, b; c, z) = 1 + \frac{ab}{c} \frac{z}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)} \frac{z^2}{2!} + \cdots \quad (\text{F.5})$$

Some important properties of the functions  $d_{M'M}^J(\beta)$  are the symmetry relations

$$d_{M'M}^J(\beta) = d_{-M,-M'}^J(\beta), \quad (\text{F.6})$$

$$d_{M'M}^J(\beta) = (-)^{M'-M} d_{MM'}^J(\beta). \quad (\text{F.7})$$

One also has

$$d_{M'M}^J(\beta) = d_{MM'}^J(-\beta) \quad (\text{F.8})$$

and

$$d_{M'M}^J(\beta) = (-)^{J+M'} d_{M',-M}^J(\pi - \beta). \quad (\text{F.9})$$

In particular, for  $\beta = \pi$ , we have

$$d_{M'M}^J(\pi) = (-)^{J-M} \delta_{M',-M}. \quad (\text{F.10})$$

Useful recursion relations are given by [4]

$$\begin{aligned} (J+M)^{1/2} d_{M'M}^J(\beta) &= (J+M')^{1/2} d_{M'-1/2,M-1/2}^{J-1/2}(\beta) \cos \tfrac{1}{2}\beta \\ &+ (J-M')^{1/2} d_{M'+1/2,M-1/2}^{J-1/2}(\beta) \sin \tfrac{1}{2}\beta \end{aligned} \quad (\text{F.11})$$

and

$$\begin{aligned} &2[(J+M)(J+M-1)]^{1/2} d_{M'M}^J(\beta) \\ &= [(J+M')(J+M'-1)]^{1/2} (1 + \cos \beta) d_{M'-1,M-1}^{J-1}(\beta) \\ &\quad + 2(J^2 - M'^2)^{1/2} \sin \beta d_{M',M-1}^{J-1}(\beta) \\ &\quad + [(J-M')(J-M'-1)]^{1/2} (1 - \cos \beta) d_{M'+1,M-1}^{J-1}(\beta). \end{aligned} \quad (\text{F.12})$$

A few important particular values of the functions  $d_{M'M}^J$  are [4]

1) For  $J = l$  integer,

$$d_{m0}^l(\beta) = (-)^m d_{0m}^l(\beta) = \left( \frac{4\pi}{2l+1} \right)^{1/2} e^{-im\phi} Y_{lm}(\beta, \phi), \quad (\text{F.13})$$

$$d_{00}^l(\beta) = P_l(\cos \beta), \quad (\text{F.14})$$

$$d_{10}^l(\beta) = -[l(l+1)]^{-1/2} \sin \beta P'_l(\cos \beta), \quad (\text{F.15})$$

$$\begin{aligned} d_{20}^l(\beta) &= [(l-1)l(l+1)(l+2)]^{-1/2} \\ &\quad \times [2P'_{l-1}(\cos \beta) - l(l-1)P_l(\cos \beta)], \end{aligned} \quad (\text{F.16})$$

$$\begin{aligned} d_{m1}^l(\beta) &= [l(l+1)]^{-1/2} \left[ -m \left( \frac{1 + \cos \theta}{\sin \theta} \right) d_{m0}^l(\beta) \right. \\ &\quad \left. - [(l-m)(l+m+1)]^{1/2} d_{m+1,0}^l(\beta) \right], \end{aligned} \quad (\text{F.17})$$

where  $P'_l(\cos \beta) = dP_l(\cos \beta)/d(\cos \beta)$ .

2) For  $J = l + \frac{1}{2}$  half integer,

$$d_{1/2,1/2}^J(\beta) = (l+1)^{-1} \cos \tfrac{1}{2}\beta [P'_{l+1}(\cos \beta) - P'_l(\cos \beta)], \quad (\text{F.18})$$

$$d_{-1/2,1/2}^J(\beta) = (l+1)^{-1} \sin \tfrac{1}{2}\beta [P'_{l+1}(\cos \beta) + P'_l(\cos \beta)], \quad (\text{F.19})$$

$$d_{1/2,3/2}^J(\beta) = (l+1)^{-1} \sin \frac{1}{2}\beta \left[ \left( \frac{l}{l+2} \right)^{1/2} P'_{l+1}(\cos \beta) + \left( \frac{l+2}{l} \right)^{1/2} P'_l(\cos \beta) \right], \quad (\text{F.20})$$

$$d_{-1/2,3/2}^J(\beta) = (l+1)^{-1} \cos \frac{1}{2}\beta \left[ -\left( \frac{l}{l+2} \right)^{1/2} P'_{l+1}(\cos \beta) + \left( \frac{l+2}{l} \right)^{1/2} P'_l(\cos \beta) \right]. \quad (\text{F.21})$$

Finally, we note that

$$\int_0^\pi d\theta \sin \theta d_{M'M}^J(\theta) d_{M'M}^{J'}(0) = \frac{2}{2J+1} \delta_{JJ'}. \quad (\text{F.22})$$

## References and notes

- [1] See for example ROSE, M. E. (1957), *Elementary Theory of Angular Momentum* (Wiley, New York) Chapter 4.
- [2] EDMONDS, A. R. (1957), *Angular Momentum in Quantum Mechanics* (Princeton University Press) Chapter 4. Since we adopt the notation of ref. [1] it should be noted that the quantity denoted by  $d_{M'M}^J(\beta)$  in Edmond's book corresponds to  $d_{M'M}^J(-\beta) = d_{MM'}^J(\beta)$  in our case.
- [3] We use here the notation of ERDÉLYI, A., W. MAGNUS, F. OBERHETTINGER and F. G. TRICOMI (1953), *Higher Transcendental Functions* (Bateman Manuscript Project, McGraw-Hill, New York) Vol. II, Chapter 10.
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